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CRYSTAL STRUCTURES OF POLY-PARAPHENYLENE OLIGOMERS CONTAINING PENDANT PHENYL GROUPS

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The room temperature crystal structures of 1,2,4-triphenylbenzene (TPB), $C_{24}H_{18}$; 2^2, 4^5-diphenyl-p-quinquephenyl (DPQ), $C_{42}H_{30}$; and 2^2, 6^5-diphenyl-p-septiphenyl (DPS), $C_{54}H_{38}$, have been investigated as part of a research program in rigid-rod polymers, materials which are of great interest for aerospace and electro-optical applications. The molecules are non-planar, in contrast to the planar structures found at room temperature for the unsubstituted polyphenyls. The oligomer axis does not align with any of the crystallographic axes. The pendant-oligomer bond, however, does align with the longest crystallographic axis. The pendant torsion angle is greater than 45° and increases with increasing chain length. Knowledge of molecular structure and crystal packing of oligomeric model compounds will be useful in further calculations of mechanical, optical, and elctro-optical properties for the corresponding rigid-rod polymer structures.

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FORWORD

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SECTION I

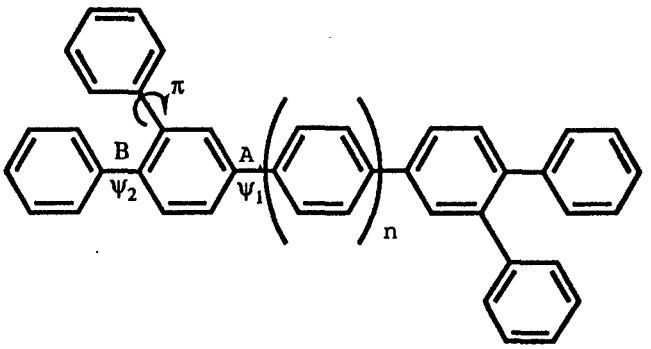
INTRODUCTION

The past few years have seen the activity in the area of conducting polymers grow at a very rapid rate. The widespread interest in conducting polymers clearly reflects their perceived technological potential[1]. Attention has focused on the pi-bonded polymers such as poly-paraphenylene (PPP) because (1) it can be oxidized to a polymeric cation rather than undergo other chemistry and thereby be made electrically conducting, (2) it is thermally stable, (3) pi-orbital overlap may create interesting non-linear optical (NLO) properties, and (4) improved methods have been reported for the synthesis of oligomeric soluble prepolymer[2].

The generation of charge carriers in the polyphenyls occurs by doping and the subsequent formation of ionic species, e.g., a polymeric cation and a counterion. Electrical conductivity as high as 500 $(ohm\ cm)^{-1}$ has been achieved with dopants such as Li, K, and AsF_5[3]. The polymer chains, as for organic molecules in general, adopt a different conformation in the ionized state compared to the neutral state. Conformation differences would lead to changes in the amount of pi-orbital overlap along the polymer axis as well as affect the electro-optical properties of the polymer.

In an ongoing study of PPP as new electrically conducting rigid-rod polymers, the room temperature

structures of $2^2,4^5$-diphenyl-p-quinquephenyl (DPQ), $2^2,6^5$-diphenyl-p-septiphenyl (DPS), and 1,2,4-triphenylbenzene (TPB) have been determined. TPB was included in this present study since its room temperature crystal structure had not been reported. The first two compounds have the general structure,



where n=1 for DPQ and n=3 for DPS. Letters (A, B, etc.) refer to the connecting bond along the main chain and the Greek letters (π and Ψ) refer to the torsion angles between adjacent phenyl groups. These compounds were synthesized in order to obtain a better understanding of how rigid rod molecules pack in solids and how chain length affects packing. In addition, recent calculations[4] have indicated that PPP is a very stiff molecule which, if processed into fibers using high molecular weight polymer, would have very high tensile modulus.

SECTION II

EXPERIMENTAL METHODS

Oligomers were synthesized by Bruce Reinhardt, Materials Laboratory, Wright Patterson Air Force Base, according to a new method utilizing intermolecular cyclization[2]. The highly crystalline samples required no additional purification and/or crystal growth. Density measurements were made by flotation in mixed solvents containing methyl alcohol and methylene chloride.

Reflection data were collected on an Enraf Nonus CAD4 diffractometer coupled with a DEC micro PDP-11 computer and processed on a VAX 11/730 using software in the Structure Determination Package (SDP)[5]. Structure solutions were determined by MULTAN 11/82[6] and SHELXS-86[7]. The method of refinement followed the general scheme: (1) Isotropic refinement of carbon atoms using unit-weighted reflections; (2) Isotropic refinement of carbon atoms using unit-weighted reflections; hydrogen atoms, with fixed thermal factors, positioned in idealized geometries and constrained to its attached carbon atom with a bond length of 0.95 Å; (3) Anisotropic refinement of carbon atoms using unit weights with hydrogen atoms still constrained to attached carbon atoms; and (4) Anisotropic refinement of carbon atoms to convergence using $1/\sigma^2(F)$ weights with hydrogen atoms riding on attached carbon atoms. Subsequent isotropic refinement of

hydrogen atoms, as expected, did not yield appreciably better results because of the reduced data-to-parameter ratio.

SECTION III

RESULTS

Table I lists crystallographic and data collection parameters, and final refinement results. Figure 1 shows the TPB molecule with the carbon atoms labeled. Tables II and III contain the atomic positions, bond distances, and bond angles, respectively. Figure 2 shows a stereoview of the molecular packing in the unit cell.

DPQ is shown in Figure 3 with the carbon atoms of the asymmetric unit labeled. Tables IV and V present the atomic positions, bond distances, and bond angles, respectively. The stereoview of the molecular packing in the unit cell is shown in Figure 4. The molecule possesses a center of symmetry.

The DPS molecule with the carbon atoms of the asymmetric unit labeled is shown in Figure 5. Atomic positions, bond distances, and bond angles are presented in Tables VI and VII, respectively. Figure 6 depicts a stereoview of the molecular packing of the structure in the unit cell. This molecule also possesses a center of symmetry.

TABLE I

CRYSTAL DATA

Name	1,2,4-Triphenyl Benzene	2^2,4^5-Diphenyl-p-quinquephenyl	2^2,6^5-Diphenyl-p-septiphenyl
Formula	$C_{24}H_{18}$	$C_{42}H_{30}$	$C_{54}H_{38}$
FW	306.41	534.7	686.9
T_m,°C	123	288	375
Crystal System	Orthorhombic	Monoclinic	Triclinic
Space Group	Pbca	$P2_1/c$	$P\bar{1}$
Z	8	2	1
a,A	10.368(6)	6.304(3)	11.713(2)
b,A	17.898(4)	31.437(9)	13.596(2)
c,A	18.474(5)	7.651(3)	6.138(2)
α,degrees	90.0	90.0	102.33(2)
β,degrees	90.0	106.18(4)	96.51(2)
γ,degrees	90.0	90.0	102.71(1)
Vol,A^3	3428.3(38)	1456.4(19)	918.3(8)
Density$_{cal}$, g/cm^3	1.187	1.219	1.242
Density$_{exp}$, g/cm^3	1.186	1.188	1.236
Crystal Dimensions, mm	0.74x0.69x0.50	0.10x0.15x0.70	0.10x0.20x0.40
Crystal Shape	Distorted octagon	Long needle	Flat needle
Cell determined	25 reflections $8°<2\theta<20°$	25 reflections $8°<2\theta<18°$	25 reflections $4°<2\theta<22°$
Radiation	Mo(graphite)	Mo(graphite)	Mo(graphite)
Scan type	$\omega/2\theta$	$\omega/2\theta$	$\omega/2\theta$
Scan rate, deg./min.	1.27-5.49	1.27-5.49	1.27-5.49

TABLE I (Continued)

	TPB	DPQ	DPS
Scan angle, degrees	0.80+0.34Tanθ	0.80+0.34Tanθ	0.80+0.34Tanθ
Power	45Kv/20ma	45Kv/20ma	45Kv/20ma
Collimator	0.8mm	0.4mm	0.4mm
Detector aperture	4.00mm	4.00mm	4.00mm
Check reflections	3 every 200 refl. $9°<2\theta<10°$	4 every 200 refl. $8°<2\theta<18°$	3 every 200 refl. $4°<2\theta<9°$
Orientation reflections	3 every 2 hours $8°<2\theta<17°$	4 every 2 hours $8°<2\theta<18°$	3 every 2 hours $8°<2\theta<13°$
Temp., °C	22	22	22
2θ range, degrees	2-60°	2-50°	2-50°
Data collected h,k,l	$\pm$14,$\pm$25,-9-26	$\pm$7,0-37,$\pm$9	$\pm$13,$\pm$16,0-7
No. total reflections	19698	5204	3558
No. unique reflections $>3\sigma$	1839	1061	1537
No. param. varied	217	190	244
Decay corr., average	0.94078	0.99780	0.99683
Abs. coeff., cm^{-1}	0.624	0.629	0.653
Abs. corr.	none	none	none
R*	0.036	0.049	0.046
RW*	0.050	0.061	0.062
Max. shift/error in final cycle	0.01	0.01	0.01

$$^{*}R = \frac{\sum \left| |F_o| - |F_c| \right|}{\sum |F_o|}$$

$$^{*}RW = \sqrt{\frac{\sum W\left(|F_o| - |F_c|\right)^2}{\sum W(F_o)^2}}$$

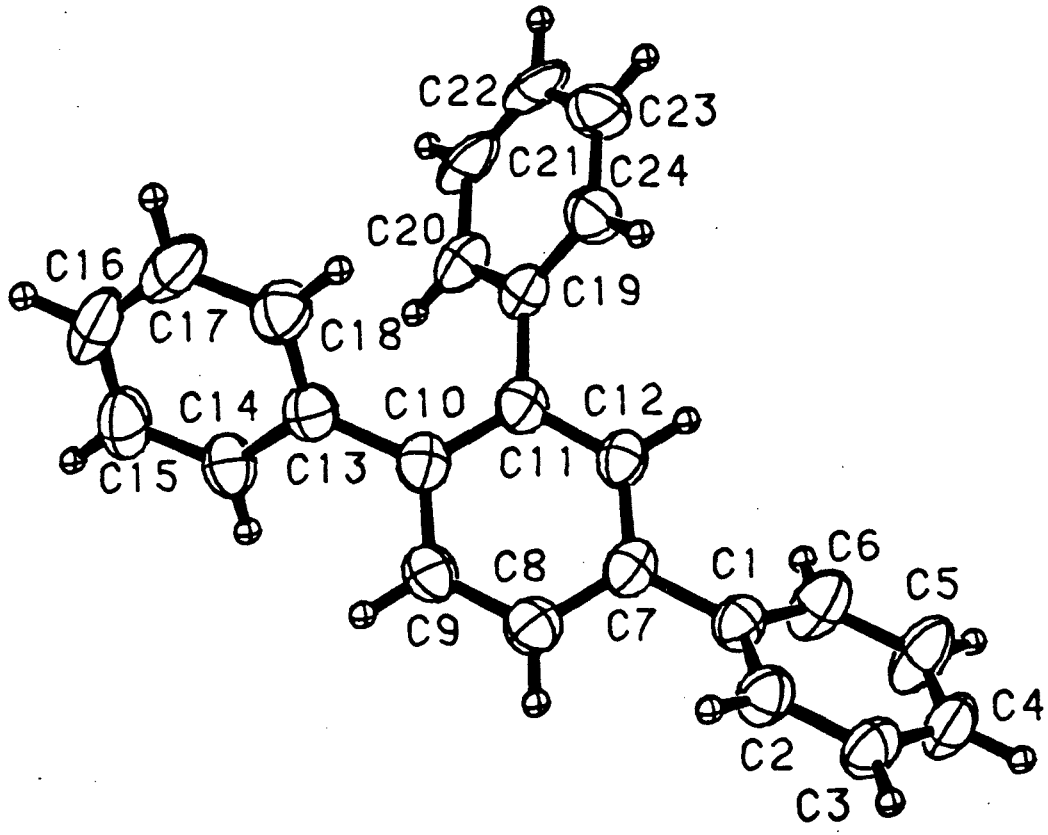


FIGURE 1. 1,2,4-Triphenylbenzene with carbon atom ellipsoids drawn at the 50% probability level.

TABLE II

Atomic Positions of
1,2,4-Triphenylbenzene

ATOM	x	y	z	B,A^2
C1	0.6605(2)	0.1066(1)	-0.02818(9)	3.51(3)
C2	0.6238(2)	0.0967(1)	-0.0998(1)	3.94(4)
C3	0.5698(2)	0.1542(1)	-0.1390(1)	4.38(4)
C4	0.5516(2)	0.2233(1)	-0.1076(1)	4.76(5)
C5	0.5875(3)	0.2341(1)	-0.0369(1)	5.76(5)
C6	0.6419(2)	0.1764(1)	0.0022(1)	5.17(5)
C7	0.7186(2)	0.0445(1)	0.01392(9)	3.46(3)
C8	0.6704(2)	-0.0279(1)	0.0092(1)	3.87(4)
C9	0.7261(2)	-0.0854(1)	0.04820(9)	3.81(4)
C10	0.8327(2)	-0.0736(1)	0.09264(9)	3.38(3)
C11	0.8815(2)	-0.0007(1)	0.09859(9)	3.34(3)
C12	0.8232(2)	0.0567(1)	0.05922(9)	3.65(4)
C13	0.8905(2)	-0.1397(1)	0.12927(9)	3.57(4)
C14	0.8133(2)	-0.1891(1)	0.1676(1)	4.24(4)
C15	0.8641(2)	-0.2526(1)	0.1991(1)	5.05(5)
C16	0.9928(3)	-0.2682(1)	0.1922(1)	5.53(5)
C17	1.0707(2)	-0.2197(1)	0.1547(1)	5.53(5)
C18	1.0206(2)	-0.1558(1)	0.1236(1)	4.49(4)
C19	0.9919(2)	0.01889(9)	0.14651(9)	3.41(4)
C20	0.9958(2)	-0.0032(1)	0.2188(1)	4.26(4)
C21	1.0960(2)	0.0181(1)	0.2634(1)	5.17(5)
C22	1.1940(2)	0.0621(1)	0.2362(1)	5.21(5)
C23	1.1915(2)	0.0842(1)	0.1647(1)	5.02(5)
C24	1.0910(2)	0.0629(1)	0.1201(1)	4.15(4)
H2	0.637	0.050	-0.122	5.0
H3	0.543	0.146	-0.188	5.6
H4	0.516	0.263	-0.135	6.0
H5	0.575	0.282	-0.015	6.9
H6	0.666	0.184	0.051	6.5
H8	0.599	-0.038	-0.022	5.0
H9	0.691	-0.134	0.045	4.8
H12	0.857	0.106	0.063	4.6
H14	0.724	-0.179	0.172	5.3
H15	0.810	-0.286	0.226	6.4
H16	1.028	-0.312	0.213	7.0
H17	1.160	-0.230	0.150	6.9
H18	1.076	-0.122	0.098	5.7
H20	0.929	-0.034	0.237	5.4
H21	1.097	0.003	0.313	6.6
H22	1.263	0.077	0.267	6.5
H23	1.260	0.114	0.146	6.6
H24	1.089	0.079	0.071	5.4

Numbers in parentheses are estimated standard deviations in the least significant digits.

TABLE III

Bond Distances and Angles for
1,2,4-Triphenylbenzene

Atom 1	Atom 2	Distance,Å	Atom 1	Atom 2	Distance,Å
C1	C2	1.388(2)	C11	C12	1.396(3)
C1	C6	1.382(3)	C11	C19	1.489(2)
C1	C7	1.486(2)	C13	C14	1.387(3)
C2	C3	1.377(3)	C13	C18	1.383(3)
C3	C4	1.379(3)	C14	C15	1.382(3)
C4	C5	1.373(3)	C15	C16	1.369(3)
C5	C6	1.381(3)	C16	C17	1.373(3)
C7	C8	1.392(3)	C17	C18	1.382(4)
C7	C12	1.387(2)	C19	C20	1.394(3)
C8	C9	1.383(3)	C19	C24	1.384(3)
C9	C10	1.393(3)	C20	C21	1.380(4)
C10	C11	1.405(2)	C21	C22	1.381(3)
C10	C13	1.489(2)	C22	C23	1.380(3)
			C23	C24	1.382(2)

Atom 1	Atom 2	Atom 3	Angle,°	Atom 1	Atom 2	Atom 3	Angle,°
C2	C1	C6	117.8(2)	C12	C11	C19	118.0(2)
C2	C1	C7	121.0(2)	C7	C12	C11	122.5(2)
C6	C1	C7	121.3(2)	C10	C13	C14	120.4(2)
C1	C2	C3	121.2(2)	C10	C13	C18	121.5(2)
C2	C3	C4	120.4(2)	C14	C13	C18	118.0(2)
C3	C4	C5	119.4(2)	C13	C14	C15	121.2(2)
C4	C5	C6	120.2(3)	C14	C15	C16	120.0(2)
C1	C6	C5	121.3(2)	C15	C16	C17	119.4(3)
C1	C7	C8	121.2(2)	C16	C17	C18	120.9(2)
C1	C7	C12	121.1(2)	C13	C18	C17	120.4(4)
C8	C7	C12	117.7(2)	C11	C19	C20	121.7(2)
C7	C8	C9	120.6(2)	C11	C19	C24	119.7(2)
C8	C9	C10	121.8(2)	C20	C19	C24	118.6(2)
C9	C10	C11	118.2(2)	C19	C20	C21	121.0(2)
C9	C10	C13	117.9(2)	C20	C21	C22	119.7(2)
C11	C10	C13	123.9(2)	C21	C22	C23	120.0(2)
C10	C11	C12	119.2(2)	C22	C23	C24	120.4(2)
C10	C11	C19	122.9(2)	C19	C24	C23	120.4(2)

Numbers in parentheses are estimated standard deviations in the least significant digit.

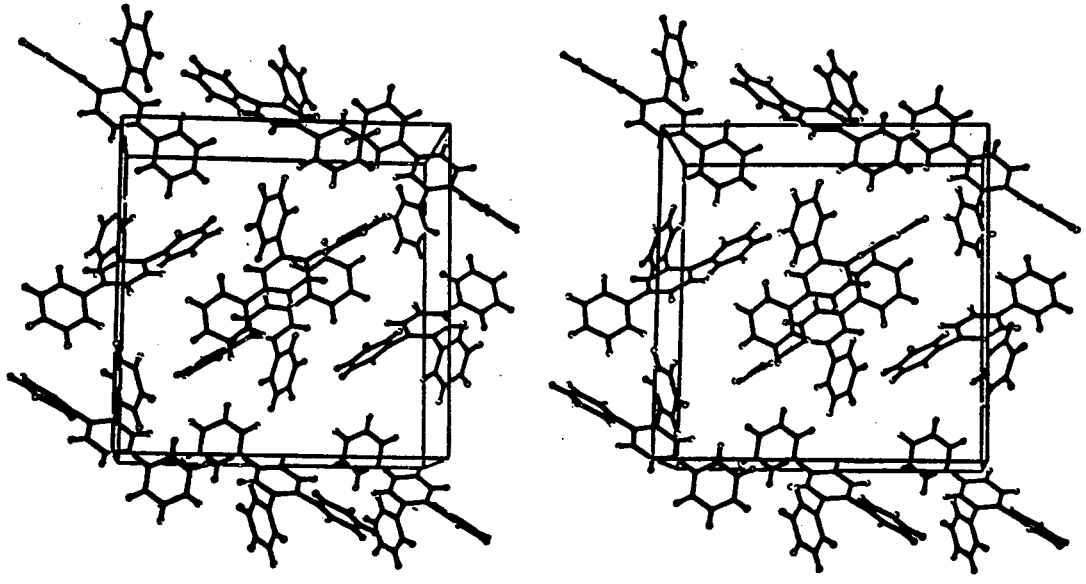


FIGURE 2. Stereoview of the partial contents of the unit cell of TPB. Molecules positioned on front corners are omitted for clarity. The b axis is horizontal and the c axis is vertical.

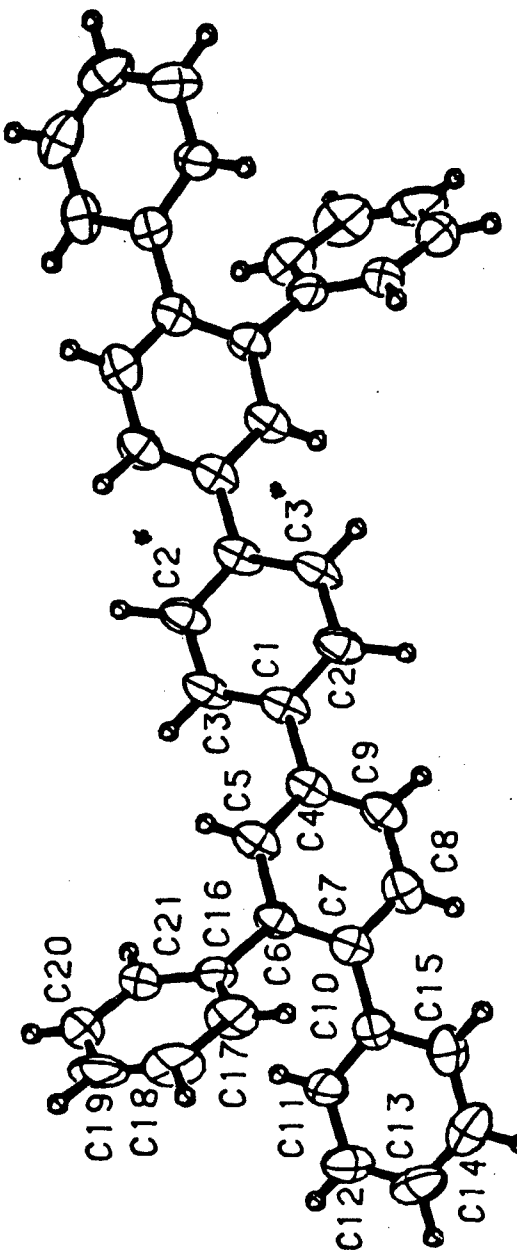


FIGURE 3. $2^2,4^5$-Diphenyl-p-quinquephenyl with carbon atom ellipsoids drawn at the 50% probability level.

TABLE IV

Atomic Positions of
$2^2,4^5$-Diphenyl-p-quinquephenyl

ATOM	x	y	z	B,Å^2
C1	0.8032(5)	0.0213(1)	0.9088(4)	3.68(7)
C2	1.1965(5)	0.0219(1)	1.0586(5)	4.48(8)
C3	1.0016(5)	0.0428(1)	0.9683(5)	4.40(8)
C4	0.5973(5)	0.0439(1)	0.8084(4)	3.67(7)
C5	0.5685(5)	0.0868(1)	0.8359(4)	3.79(7)
C6	0.3824(5)	0.1093(1)	0.7367(4)	3.42(7)
C7	0.2203(5)	0.0877(1)	0.6023(4)	3.67(7)
C8	0.2476(5)	0.0446(1)	0.5776(4)	4.25(8)
C9	0.4317(5)	0.0227(1)	0.6801(5)	4.22(8)
C10	0.0256(5)	0.1101(1)	0.4820(4)	3.66(7)
C11	0.0476(5)	0.1467(1)	0.3885(5)	4.51(8)
C12	-0.1353(6)	0.1669(1)	0.2777(5)	5.3(1)
C13	-0.3438(6)	0.1512(1)	0.2611(5)	5.4(1)
C14	-0.3688(6)	0.1145(1)	0.3490(5)	5.37(9)
C15	-0.1869(5)	0.0937(1)	0.4609(5)	4.48(8)
C16	0.3637(5)	0.1548(1)	0.7810(4)	3.83(8)
C17	0.1831(6)	0.1700(1)	0.8328(5)	4.92(9)
C18	0.1711(7)	0.2117(1)	0.8807(6)	6.2(1)
C19	0.3376(7)	0.2395(1)	0.8793(6)	6.6(1)
C20	0.5186(7)	0.2252(1)	0.8288(6)	6.0(1)
C21	0.5316(6)	0.1832(1)	0.7798(5)	4.70(9)
H2	0.665	-0.044	0.874	4.0
H3	1.004	0.073	0.947	5.2
H5	0.678	0.101	0.926	4.5
H8	0.138	0.030	0.488	5.5
H9	0.445	-0.007	0.663	5.5
H11	0.191	0.158	0.402	5.3
H12	-0.117	0.192	0.212	6.4
H13	-0.471	0.166	0.190	6.9
H14	-0.512	0.103	0.333	6.5
H15	-0.206	0.069	0.524	5.8
H17	0.066	0.151	0.835	6.0
H18	0.048	0.222	0.917	7.9
H19	0.330	0.268	0.914	8.2
H20	0.633	0.245	0.825	7.1
H21	0.657	0.173	0.746	5.6

Numbers in parentheses are estimated standard deviations in the least significant digit.

TABLE V

Bond Distances and Angles for
2',4'-Diphenyl-p-quinquephenyl

Atom 1	Atom 2	Distance,Å	Atom 1	Atom 2	Distance,Å
C1	C3	1.381(4)	C8	C9	1.388(4)
C1	C2	1.380(4)	C10	C11	1.382(5)
C2	C3*	1.392(4)	C10	C15	1.401(4)
C3	C2*	1.392(4)	C11	C12	1.379(4)
C1	C4	1.490(4)	C12	C13	1.379(4)
C4	C5	1.385(4)	C13	C14	1.367(6)
C4	C9	1.386(4)	C14	C15	1.387(5)
C5	C6	1.389(5)	C16	C17	1.390(5)
C6	C7	1.405(4)	C16	C21	1.385(5)
C6	C16	1.483(4)	C17	C18	1.367(5)
C7	C8	1.385(5)	C18	C19	1.367(6)
C7	C10	1.489(4)	C19	C20	1.377(6)
			C20	C21	1.382(5)

Atom 1	Atom 2	Atom 3	Angle,°	Atom 1	Atom 2	Atom 3	Angle,°
C2	C1	C3*	117.1(4)	C4	C9	C8	120.5(3)
C1	C2	C3*	120.5(4)	C7	C10	C11	122.0(3)
C1	C3*	C2*	121.7(4)	C7	C10	C15	119.5(4)
C2	C3*	C1*	121.7(4)	C11	C10	C15	118.5(3)
C3	C2*	C1*	120.5(4)	C10	C11	C12	120.9(3)
C3	C1	C4	121.0(4)	C11	C12	C13	120.3(4)
C1	C4	C5	121.2(3)	C12	C13	C14	119.7(4)
C1	C4	C9	120.9(3)	C13	C14	C15	120.9(4)
C5	C4	C9	118.1(3)	C10	C15	C14	119.8(4)
C4	C5	C6	122.4(4)	C6	C16	C17	121.5(4)
C5	C6	C7	118.8(4)	C6	C16	C21	120.7(3)
C5	C6	C16	118.1(3)	C17	C16	C21	117.9(3)
C7	C6	C16	123.0(3)	C16	C17	C18	121.1(5)
C6	C7	C8	118.7(4)	C17	C18	C19	120.7(4)
C6	C7	C10	122.1(3)	C18	C19	C20	119.4(4)
C8	C7	C10	119.4(4)	C19	C20	C21	120.3(4)
C7	C8	C9	121.6(3)	C16	C21	C20	120.7(4)

Numbers in parentheses are estimated standard deviations in the least significant digit.

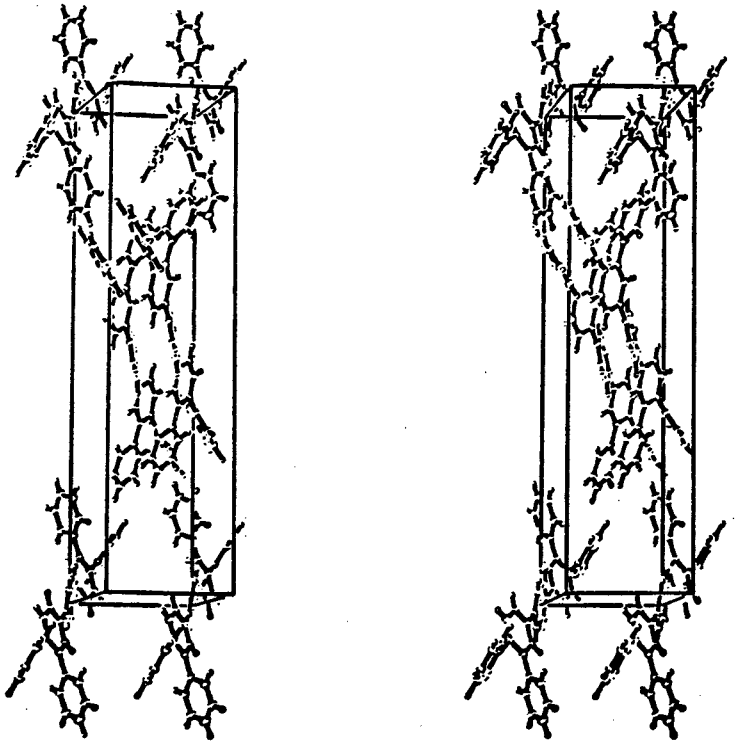


FIGURE 4. Stereoview of DPQ showing molecular packing in unit cell. Molecules positioned on front corners are omitted for clarity. The c axis is horizontal and the b axis is vertical.

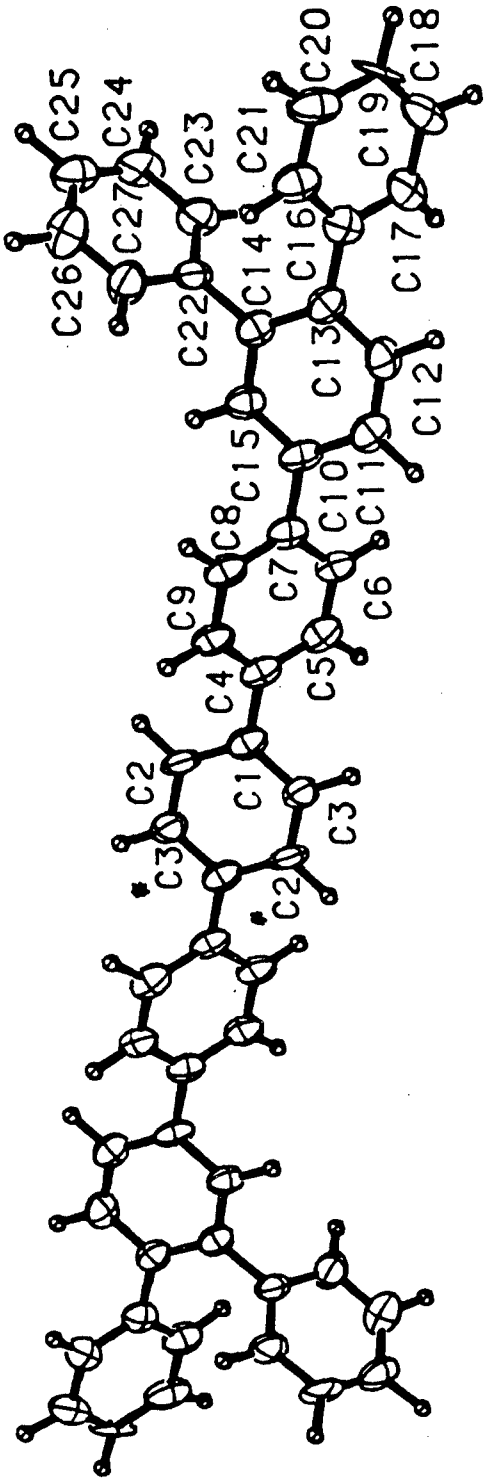


FIGURE 5. $2^2,6^5$-Diphenyl-p-septiphenyl with carbon atom ellipsoids drawn at the 50% probability level.

TABLE VI

Atomic Positions of
$2^2,6^5$-Diphenyl-p-septiphenyl

ATOM	x	y	z	B,Å^2
C1	0.5955(2)	0.5334(2)	0.3887(5)	3.77(6)
C2	0.5515(3)	0.6040(2)	0.5322(5)	4.39(7)
C3	0.5417(3)	0.4279(2)	0.3591(5)	4.35(7)
C4	0.6961(2)	0.5681(2)	0.2739(4)	3.68(6)
C5	0.6946(2)	0.5225(2)	0.0484(5)	4.14(7)
C6	0.7882(2)	0.5537(2)	-0.0607(5)	4.02(7)
C7	0.8867(2)	0.6335(2)	0.0543(4)	3.64(6)
C8	0.8885(2)	0.6795(2)	0.2815(5)	4.00(7)
C9	0.7949(2)	0.6472(2)	0.3898(5)	3.96(7)
C10	0.9859(2)	0.6701(2)	-0.0632(4)	3.72(6)
C11	1.0330(2)	0.6003(2)	-0.2050(5)	4.10(7)
C12	1.1240(2)	0.6361(2)	-0.3156(5)	4.02(7)
C13	1.1701(2)	0.7422(2)	-0.2927(5)	3.71(6)
C14	1.1220(2)	0.8133(2)	-0.1541(4)	3.64(6)
C15	1.0324(2)	0.7763(2)	-0.0412(5)	3.79(6)
C16	1.2689(2)	0.7753(2)	-0.4146(5)	3.87(6)
C17	1.2621(3)	0.7288(2)	-0.6430(5)	4.42(7)
C18	1.3543(3)	0.7581(2)	-0.7584(5)	5.70(8)
C19	1.4544(3)	0.8336(2)	-0.6477(6)	6.00(9)
C20	1.4637(3)	0.8798(2)	-0.4215(6)	5.67(9)
C21	1.3727(2)	0.8515(2)	-0.3039(5)	4.57(7)
C22	1.1624(2)	0.9279(2)	-0.1274(5)	3.77(6)
C23	1.1510(3)	0.9711(2)	-0.3105(5)	4.89(8)
C24	1.1891(3)	1.0774(2)	-0.2842(6)	5.77(9)
C25	1.2395(3)	1.1418(2)	-0.0761(6)	5.46(8)
C26	1.2498(3)	1.1005(2)	0.1086(6)	5.63(9)
C27	1.2106(3)	0.9936(2)	0.0831(5)	4.86(8)
H2	0.584	0.686	0.542	4.0
H3	0.581	0.376	0.252	4.0
H5	0.616	0.461	-0.056	5.3
H6	0.780	0.520	-0.236	5.1
H8	0.965	0.737	0.377	5.1
H9	0.801	0.681	0.560	5.0
H11	0.999	0.519	-0.223	5.3
H12	1.164	0.586	-0.415	5.3
H15	1.001	0.828	0.064	4.8
H17	1.188	0.679	-0.719	5.7
H18	1.337	0.717	-0.932	7.4
H19	1.520	0.852	-0.735	7.6
H20	1.536	0.938	-0.309	7.2
H21	1.378	0.882	-0.126	6.0
H23	1.105	0.920	-0.476	6.0
H24	1.172	1.102	-0.430	7.4
H25	1.274	1.230	-0.048	6.8
H26	1.291	1.148	0.283	7.1
H27	1.221	0.967	0.224	6.1

Numbers in parentheses are estimated standard deviations in the least significant digit.

TABLE VII

Bond Distances and Angles for
$2^2,6^5$-Diphenyl-p-septiphenyl

Atom 1	Atom 2	Distance,Å	Atom 1	Atom 2	Distance,Å
C1	C2	1.387(4)	C13	C14	1.404(4)
C1	C3*	1.397(3)	C13	C16	1.487(5)
C2	C3*	1.380(4)	C14	C15	1.384(4)
C3	C2*	1.380(4)	C14	C22	1.493(3)
C1	C4	1.481(4)	C16	C17	1.395(4)
C4	C5	1.387(4)	C16	C21	1.404(3)
C4	C9	1.393(4)	C17	C18	1.390(5)
C5	C6	1.383(4)	C18	C19	1.372(4)
C6	C7	1.394(4)	C19	C20	1.378(5)
C7	C8	1.397(4)	C20	C21	1.384(5)
C7	C10	1.486(4)	C22	C23	1.382(4)
C8	C9	1.384(4)	C22	C27	1.380(4)
C10	C11	1.395(4)	C23	C24	1.384(4)
C10	C15	1.399(3)	C24	C25	1.386(4)
C11	C12	1.382(5)	C25	C26	1.374(5)
C12	C13	1.395(4)	C26	C27	1.393(4)

Atom 1	Atom 2	Atom 3	Angle,°	Atom 1	Atom 2	Atom 3	Angle,°
C2	C1	C3	117.1(3)	C12	C13	C14	118.7(3)
C2	C1	C4	121.5(2)	C12	C13	C16	118.6(2)
C3	C1	C4	121.4(2)	C14	C13	C16	122.8(2)
C1	C4	C5*	120.9(2)	C13	C14	C15	119.3(2)
C1	C2	C3*	121.8(2)	C13	C14	C22	122.2(2)
C1	C3*	C2*	121.1(2)	C15	C14	C22	118.5(2)
C2	C3*	C1*	121.1(2)	C10	C15	C14	122.4(3)
C3	C2*	C1*	121.8(2)	C13	C16	C17	120.5(3)
C1	C4	C9	120.9(2)	C13	C16	C21	121.6(2)
C5	C4	C9	118.2(3)	C17	C16	C21	117.8(3)
C4	C5	C6	121.5(2)	C16	C17	C18	121.1(2)
C5	C6	C7	120.3(2)	C17	C18	C19	120.1(3)
C6	C7	C8	118.2(3)	C18	C19	C20	119.9(3)
C6	C7	C10	120.8(2)	C19	C20	C21	120.8(2)
C8	C7	C10	121.0(2)	C16	C21	C20	120.3(3)
C7	C8	C9	121.1(3)	C14	C22	C23	121.2(2)
C4	C9	C8	120.6(2)	C14	C22	C27	120.4(3)
C7	C10	C11	121.6(2)	C23	C22	C27	118.4(2)
C7	C10	C15	120.7(2)	C22	C23	C24	120.9(2)
C11	C10	C15	117.7(3)	C23	C24	C25	120.5(3)
C10	C11	C12	120.6(2)	C24	C25	C26	119.5(3)
C11	C12	C13	121.4(3)	C25	C26	C27	120.1(3)
				C22	C27	C26	120.6(4)

Numbers in parentheses are estimated standard deviations in the least significant digit.

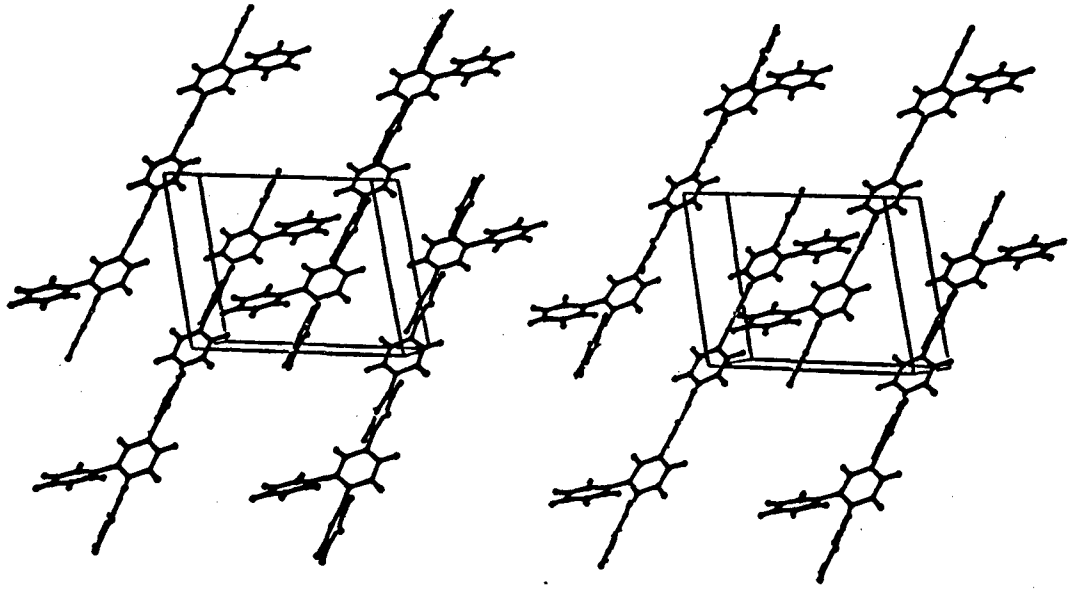


FIGURE 6. The c axis stereoview of DPS showing molecular packing in unit cell. Molecules on rear corners are omitted for clarity. The a axis is horizontal.

SECTION IV

DISCUSSION

Table VIII summarizes the bond lengths between neighboring phenyl units for structures determined at room temperature. The values are not significantly different than the corresponding distances in the unsubstituted PPP[8-11]. A significant shortening of these bond distances in the substituted oligomers would have indicated more double bond character and increased electron delocalization. The contribution of the quinoid resonance structure is believed to increase upon doping of PPP[3] with alkali metals. This is accompanied by a decrease in aromaticity and an increase in electron delocalization. Thus, it is inconclusive whether pendant-containing PPP could therefore be doped with alkali metal ions to produce better electronic conductors and/or NLO materials.

The bond angles are very close to the expected 120° value with the largest deviations in angles associated with connecting phenyl units. The oligomer axis of each molecule is essentially coaxial and small deviations are probably due to steric hindrance of the phenyl pendant groups. Deviations of the oligomer axis carbon atoms from the best least squares line fit, plotted in Figure 7, show that DPS is distorted the most of the three oligomers. When viewed down the chain axis, DPQ has a small sinusoidal-shaped wave perpendicular to the plane of the central ring, whereas TPB and DPS are bowed.

TABLE VIII

Summary of Bond Lengths Between Phenyl Units* Measured at Room Temperature

Compound Name	A,Å	B,Å	C,Å	π,Å	Conform.
Biphenyl[9]	1.495(5)	----	----	----	P
p-Terphenyl[10]	1.505(5)	----	----	----	P
p-Quaterphenyl[11]	1.502(4)	1.486(5)	----	----	P
p-Quinquephenyl[12]	1.481(5)	1.482(5)	----	----	P
p-Sexiphenyl[12]	1.506(6)	1.501(8)	1.461(8)	----	P
1,2,4-Triphenyl-benzene	1.486(2)	1.489(2)	----	1.489(2)	N
$2^2,4^5$-Diphenyl-p-quinquephenyl	1.490(4)	1.489(4)	----	1.483(4)	N
$2^2,6^5$-Diphenyl-p-septiphenyl	1.481(4)	1.486(4)	1.487(5)	1.493(3)	N

Numbers in parentheses are estimated standard deviations in the least significant digit. P means planar conformation and N means non-planar conformation.

*Nomenclature of the phenyl links is relative to the center of symmetry in the molecule such that the phenyl link is that bond which lies on the symmetry center or the nearest phenyl link if the symmetry center exists at a phenyl unit (see general structure).

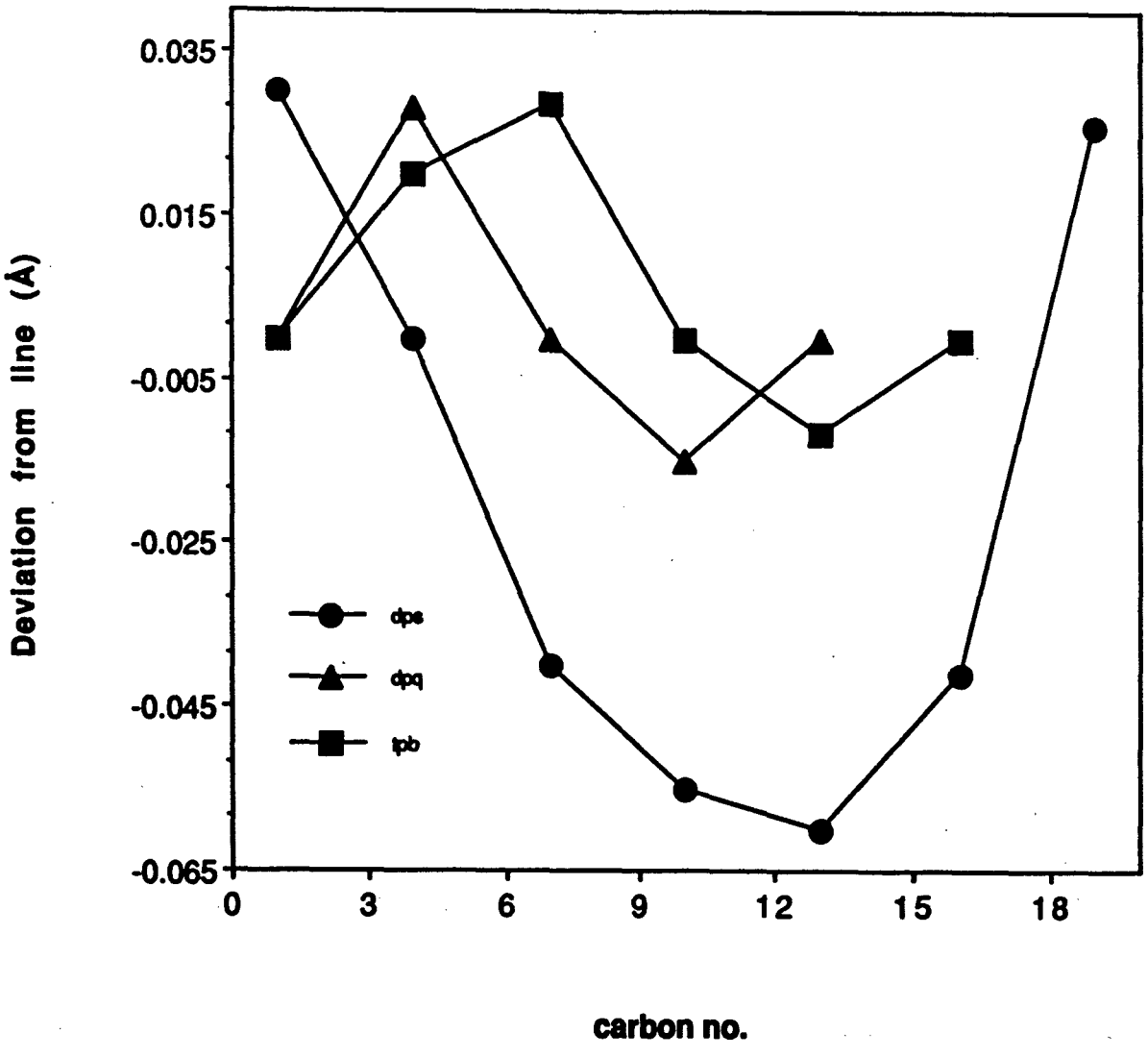


FIGURE 7. Deviation of the carbon atoms composing the oligomer axis from least squares line.

The terminal phenyl ring of TPB (C13 - C18) is 7° from being collinear with the oligomer axis. These contortions of the oligomer axis are shown in Figure 8.

In all three oligomers, the oligomer axis does not align with any of the crystallographic axes; however, the bond connecting the pendant to the oligomer aligns preferentially along (or nearly so) one of the crystallographic axes. In TPB the pendant-oligomer bond aligns close to **a**, while the pendant-oligomer bond in DPQ and DPS aligns approximately parallel to the **b** axis. In results to be published, para-quinquephenyl and para-sexiphenyl have their oligomer axes preferentially aligning with **b**[12]. Thus, with TPB being the exception, the pendant-oligomer bond aligns with the longest crystallographic axis. TPB's short chain axis and lack of molecular symmetry appear to play an important role in this alignment.

The addition of the phenyl pendant groups disrupts the planarity of the polyphenyls observed in the room temperature structures of biphenyl[13], para-terphenyl[14], para-quaterphenyl[11], para-quinquephenyl and para-sexiphenyl[12], as seen in Tables IX and X. This is most probably due to steric hindrance of the pendant groups with the oligomer chain and crystal packing forces. Hydrogen-to-hydrogen distances between phenyl rings (H2 - H9 in DPS, for example) are approximately equal to 2.5 Å. Hydrogen atoms on the terminal phenyl ring closest to the pendant group are approximately equi-distant from one of the ortho hydrogen atoms on the

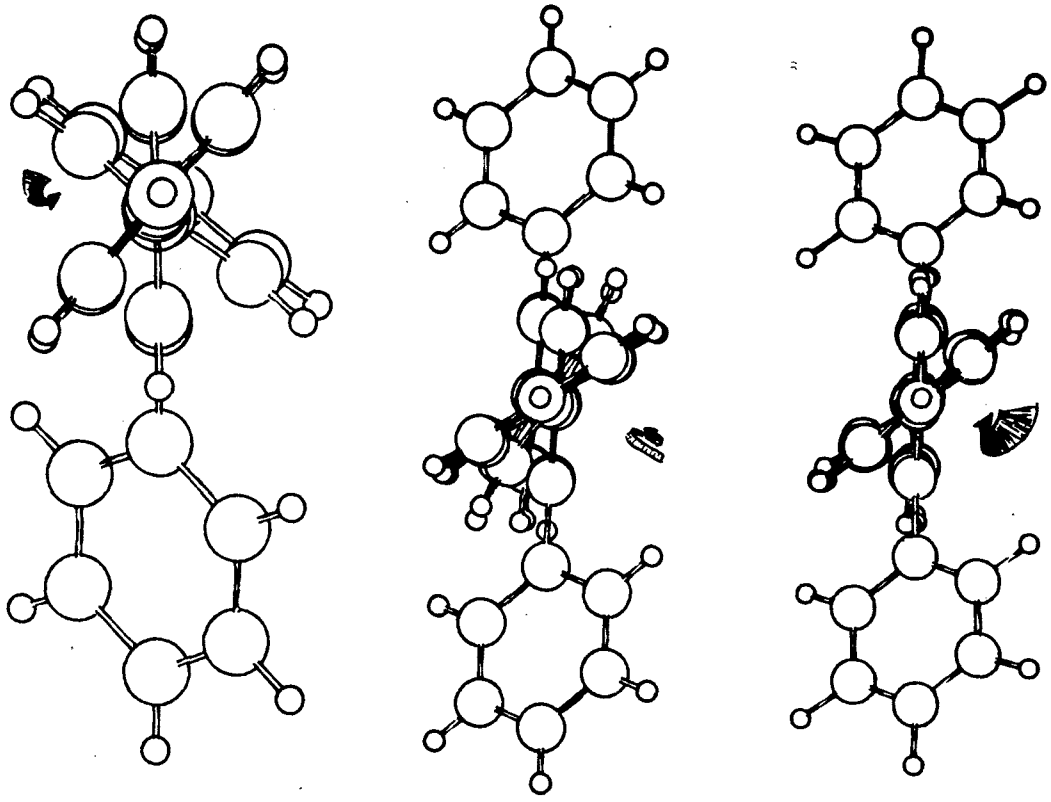


FIGURE 8. View down oligomer axes of TPB, DPQ, and DPS showing tortuosity of axis.

TABLE IX

Torsion Angles* of Straight Chain Polyphenyls

Name	Formula	Temp., K	Ψ_1, °	Ψ_2, °	Ψ_3, °
Biphenyl	$C_{12}H_{10}$	298[13]	0	---	---
		40[9]	10	---	---
p-Terphenyl	$C_{18}H_{14}$	298[14]	0	---	---
		110[15]	16	---	---
p-Quaterphenyl	$C_{24}H_{18}$	298[11]	0	0	---
		110[16]	17.1	22.7	---
p-Quinquephenyl	$C_{30}H_{22}$	298[12]	0	0	---
		110	Work in progress		
p-Sexiphenyl	$C_{36}H_{26}$	298[12]	0	0	0
		110	Work in progress		
p-Septiphenyl	$C_{42}H_{30}$	298	Work in progress		
		110	Work in progress		

*The torsion angles are labeled relative to the symmetry center of the molecule; such that, if a symmetry center exists on the bond connecting two phenyl units the torsion angle refers to the two adjacent rings. If a center of symmetry exists in a phenyl unit the torsion angle refers to the nearest chain link (see general structure).

TABLE X

Torsion Angles* of Pendant Polyphenyls

Name	Formula	Temp., K	Ψ_1, °	Ψ_2, °	Ψ_3, °	π, °
1,2,4-Triphenyl-benzene	$C_{24}H_{18}$	298	42.8	49.8	---	48.4
		110	Work in progress			
$2^2,3^5$-Diphenyl-p-quaterphenyl	$C_{36}H_{26}$	298	Work in progress			
		110	Work in progress			
$2^2,4^5$-Diphenyl-p-quinquephenyl	$C_{42}H_{30}$	298	-28.0	51.2	---	55.7
		110	Work in progress			
$2^2,5^5$-Diphenyl-p-sexiphenyl	$C_{48}H_{34}$	298	Work in progress			
		110	Work in progress			
$2^2,6^5$-Diphenyl-p-septiphenyl	$C_{54}H_{38}$	298	43.2	-45.6	48.6	61.0
		110	Work in progress			

*The torsion angles are labeled relative to the symmetry center of the molecule; such that, if a symmetry center exists on the bond connecting two phenyl units the torsion angle refers to the two adjacent rings. If a center of symmetry exists in a phenyl unit the torsion angle refers to the nearest chain link. Pendant refers to the torsion angle between the pendant group and the phenyl group to which it is attached (see general structure).

pendant group. In DPQ, for example, H11 and H15 on the terminal phenyl ring are both approximately 3.6 Å from H17 on the pendant ring (see Figure 9). The corresponding values in DPS are 3.7 Å. For the three pendant-substituted oligomers, the pendant hydrogen atom - to - terminal phenyl hydrogen atom contact increases with oligomer length (from approximately 3.5 Å in TPB to 3.7 Å in DPS).

The average torsion angle within the oligomer chain is 45°, which is approximately twice the value of 23° predicted for PPP from structural data and further supported by ab-initio quality quantum mechanical calculations[3]. The exception is DPQ which has torsion angles of approximately -28° at the center ring, but angles of 51° for the terminal ring. The reason for this large difference, unique to this oligomer, is not clear at this time.

The torsion angle between the pendant group and the oligomer chain is greater than 45°, increasing with chain length. As the hydrogen atoms of the main chain approach the hydrogen atoms of the pendant group, the pendant torsion angle decreases. This trend is not yet understood and more measurements on different model systems are under consideration. Fully-optimized AMPAC AM1 conformational calculations for the low energy structure of ortho-phenyl-substituted biphenyl reveal torsion angles of approximately 40°.[17] A line with a positive slope is obtained when the pendant torsion angle is plotted against the number of phenyl units in the oligomer chain (see Figure 10).

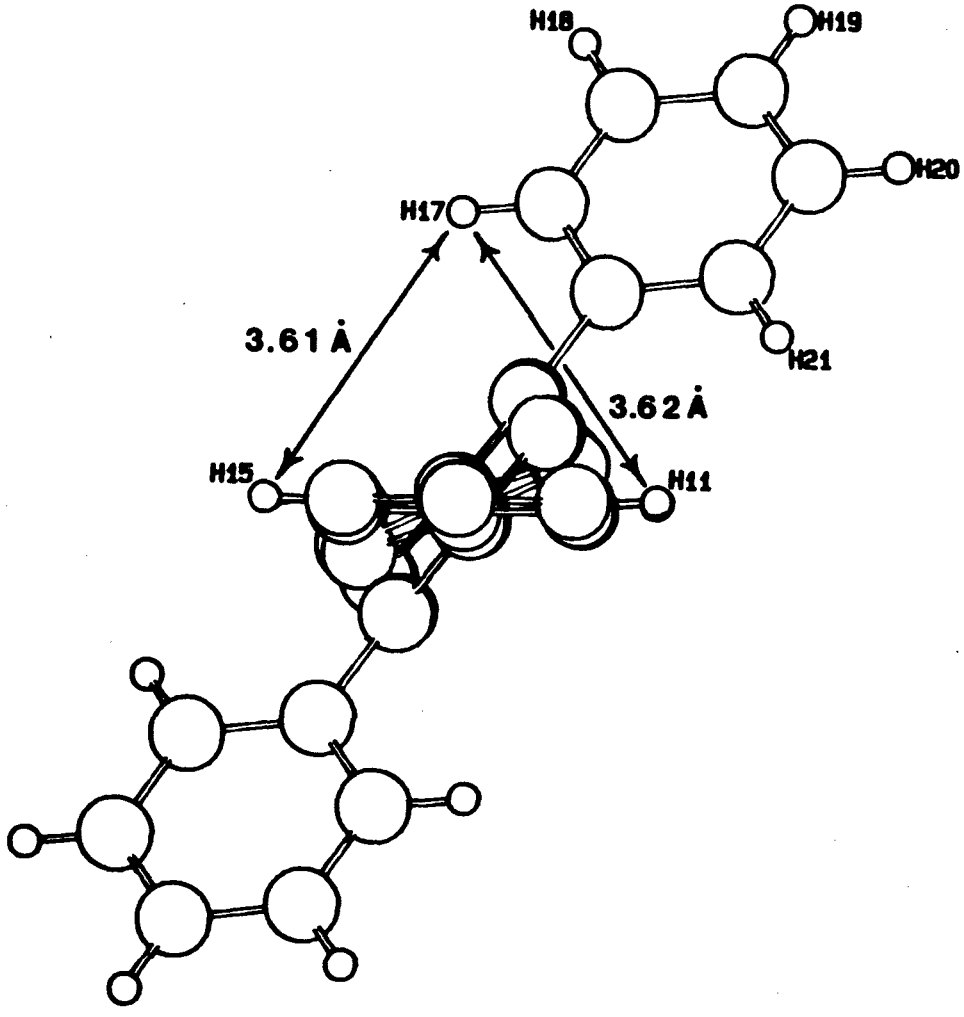


FIGURE 9. Hydrogen atom repulsion distances between pendant and oligomer axis for DPQ.

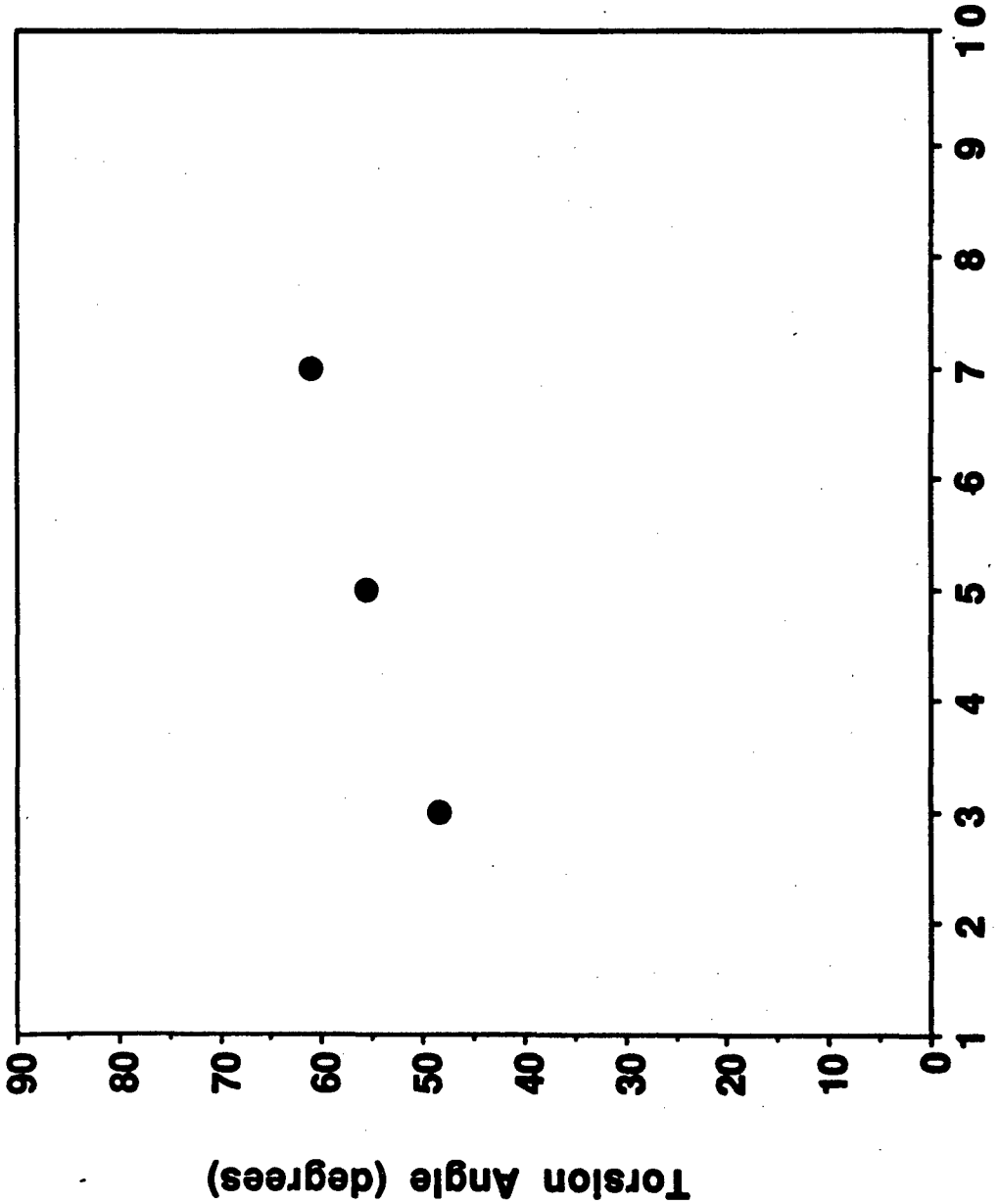


FIGURE 10. Graph of pendant torsion angle vs. total number of phenyl units in oligomer chain.

SECTION V

CONCLUSIONS

The non-planar structures of the phenyl-substituted oligomers contrast with average planar structures observed for the unsubstituted polyphenyls. The average torsion angle along the oligomer chain is 45°. The oligomer axis does not align with a crystallographic axis; however, the pendant connect bond prefers to align parallel to one of the crystallographic axes. The pendant torsion angle increases with chain length. More research is needed on oligomers with even numbers of phenyl units along the main chain to compare and contrast with those which have an odd number. Also the pendant groups of the title compounds occupy positions closest to the terminal phenyl unit. Similar measurements of compounds where the pendant group is attached closest to the central phenyl unit are needed to identify the major reasons for variations in the torsion angles along the oligomer axis.

SECTION VI

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Appendix A

Table of General Displacement Parameter Expressions - U's for 1,2,4-Triphenylbenzene

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C1	0.0447(9)	0.048(1)	0.0409(8)	0.0011(9)	0.0011(8)	0.0029(8)
C2	0.057(1)	0.048(1)	0.0446(8)	0.0021(9)	-0.0032(9)	-0.0011(9)
C3	0.067(1)	0.055(1)	0.0452(9)	0.001(1)	-0.0086(9)	0.0035(9)
C4	0.072(1)	0.051(1)	0.058(1)	0.007(1)	-0.008(1)	0.006(1)
C5	0.105(2)	0.053(1)	0.062(1)	0.020(1)	-0.009(1)	-0.007(1)
C6	0.092(2)	0.057(1)	0.0475(9)	0.013(1)	-0.010(1)	-0.006(1)
C7	0.0442(9)	0.049(1)	0.0388(7)	0.0028(8)	0.0038(8)	0.0038(8)
C8	0.0436(9)	0.054(1)	0.0490(9)	-0.0009(9)	0.0017(9)	0.0033(9)
C9	0.0464(9)	0.048(1)	0.0504(9)	-0.0045(9)	0.0023(9)	0.0043(8)
C10	0.0435(9)	0.044(1)	0.0408(8)	0.0009(8)	0.0073(8)	0.0028(7)
C11	0.0442(9)	0.046(1)	0.0366(7)	-0.0005(8)	0.0038(8)	0.0030(8)
C12	0.0500(9)	0.0441(9)	0.0409(8)	-0.0002(9)	0.0013(8)	0.0038(8)
C13	0.0499(9)	0.043(1)	0.0428(8)	-0.0004(8)	0.0004(8)	-0.0012(8)
C14	0.060(1)	0.049(1)	0.052(1)	-0.004(1)	0.004(1)	0.0056(9)
C15	0.086(2)	0.048(1)	0.057(1)	-0.001(1)	-0.001(1)	0.0079(9)
C16	0.093(2)	0.051(1)	0.065(1)	0.016(1)	-0.011(1)	0.001(1)
C17	0.066(1)	0.065(1)	0.079(1)	0.016(1)	-0.007(1)	-0.003(1)
C18	0.052(1)	0.054(1)	0.065(1)	0.004(1)	0.003(1)	0.001(1)
C19	0.0470(9)	0.039(1)	0.0432(8)	0.0040(9)	-0.0013(8)	0.0008(7)
C20	0.059(1)	0.056(1)	0.0472(9)	0.0060(9)	-0.0040(9)	0.0058(8)
C21	0.077(1)	0.065(1)	0.055(1)	0.014(1)	-0.019(1)	-0.002(1)
C22	0.065(1)	0.056(1)	0.076(1)	0.013(1)	-0.025(1)	-0.014(1)
C23	0.055(1)	0.052(1)	0.084(1)	-0.003(1)	-0.009(1)	-0.010(1)
C24	0.052(1)	0.050(1)	0.055(1)	-0.003(1)	-0.001(1)	-0.0011(9)

The form of the anisotropic displacement parameter is:
exp[-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}] where a,b, and c are reciprocal lattice constants.

Appendix A

Table of General Displacement Parameter Expressions - U's for 2',4''-Diphenyl-p-quinquephenyl

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C1	0.050(1)	0.040(2)	0.053(2)	0.007(1)	0.024(1)	0.005(1)
C2	0.050(2)	0.047(2)	0.070(2)	0.008(2)	0.016(1)	0.010(2)
C3	0.057(2)	0.036(2)	0.075(2)	0.008(2)	0.020(1)	0.011(2)
C4	0.049(2)	0.041(2)	0.051(2)	0.005(1)	0.018(1)	0.004(1)
C5	0.045(1)	0.041(2)	0.056(2)	0.005(1)	0.014(1)	0.002(1)
C6	0.044(1)	0.037(2)	0.048(2)	0.006(1)	0.010(1)	0.001(1)
C7	0.043(1)	0.045(2)	0.050(2)	0.001(1)	0.015(1)	0.002(2)
C8	0.053(2)	0.046(2)	0.056(2)	-0.002(2)	0.010(1)	-0.004(2)
C9	0.061(2)	0.037(2)	0.062(2)	0.005(2)	0.017(1)	-0.001(2)
C10	0.043(2)	0.045(2)	0.047(2)	0.001(1)	0.009(1)	-0.002(2)
C11	0.047(2)	0.055(2)	0.062(2)	-0.002(2)	0.004(2)	0.009(2)
C12	0.066(2)	0.066(2)	0.060(2)	0.007(2)	0.008(2)	0.013(2)
C13	0.052(2)	0.082(3)	0.061(2)	0.017(2)	0.001(2)	-0.004(2)
C14	0.040(2)	0.088(3)	0.067(2)	-0.003(2)	0.005(2)	-0.010(2)
C15	0.052(2)	0.056(2)	0.062(2)	-0.006(2)	0.017(1)	-0.002(2)
C16	0.047(2)	0.040(2)	0.050(2)	0.006(2)	0.001(1)	0.001(2)
C17	0.056(2)	0.055(2)	0.072(2)	0.013(2)	0.013(2)	-0.008(2)
C18	0.073(2)	0.065(2)	0.089(3)	0.024(2)	0.009(2)	-0.016(2)
C19	0.103(3)	0.048(2)	0.080(3)	0.024(2)	-0.008(2)	-0.008(2)
C20	0.076(2)	0.044(2)	0.092(3)	0.000(2)	-0.007(2)	0.001(2)
C21	0.050(2)	0.044(2)	0.073(2)	0.001(2)	0.003(2)	0.004(2)

The form of the anisotropic displacement parameter is:
exp[-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}] where a,b, and c are reciprocal lattice constants.

Table of General Displacement Parameter Expressions - U's for $2^2,6^5$-Diphenyl-p-septiphenyl

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C1	0.046(1)	0.042(1)	0.052(2)	0.006(1)	0.001(1)	0.013(1)
C2	0.058(2)	0.037(1)	0.071(2)	0.004(1)	0.015(1)	0.016(1)
C3	0.059(2)	0.038(1)	0.067(2)	0.008(1)	0.014(1)	0.011(1)
C4	0.046(1)	0.039(1)	0.053(2)	0.008(1)	0.000(1)	0.016(1)
C5	0.046(2)	0.042(1)	0.059(2)	0.001(1)	-0.001(1)	0.009(1)
C6	0.052(2)	0.043(1)	0.053(2)	0.003(1)	0.005(1)	0.012(1)
C7	0.045(1)	0.041(1)	0.052(2)	0.010(1)	0.003(1)	0.015(1)
C8	0.051(2)	0.043(1)	0.054(2)	0.006(1)	0.002(1)	0.013(1)
C9	0.052(2)	0.044(1)	0.050(2)	0.005(1)	0.002(1)	0.015(1)
C10	0.044(1)	0.042(1)	0.054(2)	0.008(1)	0.002(1)	0.018(1)
C11	0.052(2)	0.042(1)	0.059(2)	0.010(1)	0.002(1)	0.011(1)
C12	0.052(2)	0.044(1)	0.053(2)	0.014(1)	0.004(1)	0.007(1)
C13	0.047(1)	0.039(1)	0.050(2)	0.007(1)	0.002(1)	0.009(1)
C14	0.046(1)	0.038(1)	0.051(2)	0.008(1)	0.003(1)	0.010(1)
C15	0.047(1)	0.042(1)	0.053(2)	0.008(1)	0.006(1)	0.013(1)
C16	0.048(1)	0.045(1)	0.055(2)	0.014(1)	0.005(1)	0.014(1)
C17	0.059(2)	0.057(1)	0.054(2)	0.020(1)	0.010(1)	0.013(1)
C18	0.084(2)	0.074(2)	0.068(2)	0.030(1)	0.024(2)	0.022(1)
C19	0.075(2)	0.079(2)	0.093(2)	0.032(1)	0.040(2)	0.036(2)
C20	0.054(2)	0.065(2)	0.101(2)	0.015(1)	0.018(2)	0.027(2)
C21	0.047(2)	0.053(1)	0.070(2)	0.007(1)	0.005(1)	0.015(1)
C22	0.046(1)	0.039(1)	0.057(2)	0.007(1)	0.012(1)	0.012(1)
C23	0.075(2)	0.050(1)	0.063(2)	0.016(1)	0.012(2)	0.017(1)

Table of General Anisotropic Displacement Parameter Expressions - U's for $2^2,6^5$-Diphenyl-p-septiphenyl (continued)

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
C24	0.092(2)	0.054(1)	0.082(2)	0.023(1)	0.019(2)	0.029(1)
C25	0.065(2)	0.047(1)	0.099(2)	0.016(1)	0.021(2)	0.020(1)
C26	0.073(2)	0.047(2)	0.082(2)	0.009(1)	0.001(2)	0.005(2)
C27	0.072(2)	0.041(1)	0.063(2)	0.007(1)	0.003(2)	0.005(1)

The form of the anisotropic displacement parameter is:
exp[-2PI2{h2a2U(1,1) + k2b2U(2,2) + l2c2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)}] where a,b, and c are reciprocal lattice constants.

Appendix B

1,2,4-Triphenylbenzene

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
0	2	0	1188	1263	6	0	12	6	183	196	6	0	18	13	90	99	5	0	0	24	45	48	6
0	4	0	1352	1424	8	0	14	6	370	388	11	0	20	13	50	51	6	0	2	24	114	102	5
0	6	0	636	650	4	0	16	6	169	180	7	0	0	14	65	66	3	0	4	24	68	75	5
0	8	0	86	96	5	0	2	7	205	202	4	0	2	14	108	112	5	1	1	1	495	503	3
0	10	0	162	158	5	0	6	7	140	157	5	0	4	14	56	56	4	1	2	1	153	157	4
0	12	0	582	589	7	0	12	7	261	282	6	0	6	14	420	427	13	1	3	1	674	690	3
0	14	0	256	244	6	0	14	7	128	133	5	0	10	14	178	175	7	1	4	1	491	499	7
0	2	1	744	775	3	0	2	9	251	248	4	0	18	14	67	59	4	1	6	1	146	142	6
0	4	1	1730	1827	14	0	4	9	821	798	12	0	4	15	102	101	5	1	7	1	280	280	4
0	6	1	792	789	3	0	6	9	435	408	9	0	6	15	81	81	5	1	8	1	34	41	4
0	12	1	47	48	4	0	8	9	157	158	6	0	12	15	77	73	4	1	9	1	247	257	4
0	0	2	549	552	2	0	10	9	243	245	6	0	20	15	66	59	5	1	10	1	278	258	4
0	2	2	500	513	2	0	12	9	252	261	6	0	2	16	119	132	7	1	11	1	88	89	3
0	4	2	1018	1050	3	0	14	9	132	133	4	0	4	16	110	116	5	1	13	1	135	130	5
0	6	2	456	450	3	0	16	9	120	126	4	0	6	16	110	106	4	1	14	1	85	87	4
0	8	2	475	469	4	0	18	9	90	88	4	0	8	16	201	202	7	1	15	1	416	419	11
0	10	2	57	56	2	0	20	9	84	83	6	0	10	16	405	412	7	1	16	1	408	422	6
0	12	2	221	214	10	0	0	10	141	141	5	0	12	16	116	121	5	1	22	1	95	94	3
0	14	2	273	273	9	0	2	10	91	88	3	0	2	17	91	96	4	1	0	2	374	377	5
0	16	2	175	178	16	0	4	10	353	355	4	0	4	17	94	87	3	1	1	2	180	182	3
0	22	2	64	61	5	0	8	10	173	165	6	0	6	17	258	250	10	1	2	2	345	353	3
0	2	3	1760	1868	8	0	12	10	139	143	10	0	8	17	246	253	7	1	3	2	923	955	6
0	4	3	173	184	3	0	14	10	104	107	6	0	16	17	109	100	5	1	4	2	413	419	5
0	6	3	127	130	7	0	16	10	85	84	3	0	0	18	93	92	5	1	5	2	621	627	4
0	8	3	601	579	4	0	18	10	73	72	4	0	2	18	113	112	4	1	6	2	559	555	5
0	10	3	186	194	5	0	2	11	426	402	4	0	4	18	68	61	4	1	8	2	84	79	4
0	12	3	209	201	6	0	4	11	365	362	4	0	6	18	63	62	4	1	9	2	174	175	5
0	14	3	456	464	8	0	6	11	187	192	6	0	8	18	219	220	8	1	10	2	57	52	2
0	16	3	72	78	3	0	10	11	161	163	11	0	10	18	116	112	4	1	11	2	93	89	4
0	0	4	705	718	2	0	12	11	103	106	7	0	16	18	45	52	7	1	13	2	105	108	4
0	2	4	842	862	4	0	14	11	192	192	7	0	2	19	159	170	6	1	16	2	257	253	7
0	4	4	994	1030	3	0	16	11	66	64	6	0	4	19	213	220	7	1	1	3	1437	1491	18
0	8	4	116	98	4	0	20	11	76	76	4	0	8	19	93	105	4	1	2	3	1055	1083	7
0	12	4	176	180	6	0	0	12	100	101	5	0	10	19	150	155	8	1	3	3	217	214	6
0	14	4	526	543	5	0	2	12	308	306	6	0	12	19	117	130	5	1	4	3	129	128	5
0	16	4	124	125	4	0	4	12	152	147	6	0	0	20	160	160	5	1	5	3	425	431	4
0	2	5	603	620	3	0	6	12	170	172	5	0	4	20	152	159	6	1	6	3	143	152	4
0	4	5	975	989	3	0	8	12	378	381	5	0	6	20	66	64	5	1	7	3	158	158	6
0	6	5	431	426	4	0	10	12	275	280	8	0	12	20	94	90	4	1	8	3	37	40	4
0	8	5	740	728	4	0	12	12	80	78	4	0	2	21	126	132	4	1	9	3	60	52	3
0	10	5	67	67	4	0	14	12	121	122	5	0	8	21	95	96	4	1	10	3	411	410	4
0	12	5	345	365	5	0	18	12	44	44	6	0	12	21	57	56	5	1	11	3	157	152	5
0	14	5	333	337	6	0	20	12	109	99	4	0	0	22	94	97	4	1	14	3	264	270	6
0	0	6	640	647	3	0	2	13	59	58	3	0	2	22	74	61	4	1	15	3	69	63	3
0	2	6	1231	1263	7	0	4	13	161	158	6	0	6	22	98	91	5	1	16	3	125	128	5
0	4	6	112	114	4	0	6	13	204	200	6	0	12	22	99	96	4	1	0	4	557	568	5
0	6	6	446	441	4	0	8	13	308	321	5	0	4	23	56	50	6	1	1	4	1289	1336	12
0	10	6	150	140	5	0	12	13	167	174	6	0	6	23	57	56	5	1	2	4	1262	1305	7

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
1	3	4	816	842	6	1	7	7	185	183	5	1	20	11	63	51	5	1	13	16	74	77	4
1	4	4	320	322	3	1	9	7	234	237	5	1	0	12	57	54	2	1	15	16	63	58	4
1	5	4	810	819	5	1	10	7	200	194	5	1	2	12	49	41	3	1	2	17	63	70	4
1	6	4	301	308	7	1	11	7	205	211	7	1	3	12	43	48	6	1	3	17	176	185	7
1	7	4	534	527	4	1	12	7	77	72	6	1	4	12	262	253	7	1	5	17	201	213	8
1	8	4	503	498	4	1	13	7	58	56	5	1	6	12	172	167	6	1	6	17	63	64	3
1	9	4	118	120	5	1	15	7	71	66	3	1	7	12	135	145	5	1	9	17	118	120	5
1	10	4	99	100	5	1	22	7	54	55	6	1	9	12	104	108	8	1	11	17	83	85	4
1	12	4	82	80	7	1	21	8	75	66	5	1	10	12	141	141	6	1	0	18	80	84	3
1	13	4	39	40	5	1	2	9	302	298	4	1	11	12	200	202	7	1	1	18	76	81	3
1	14	4	320	320	6	1	3	9	181	168	5	1	4	13	75	75	3	1	5	18	92	92	4
1	15	4	80	80	3	1	4	9	282	280	6	1	5	13	106	108	6	1	9	18	100	104	4
1	23	4	75	71	5	1	5	9	134	146	6	1	7	13	269	274	7	1	12	18	103	111	3
1	1	5	865	879	4	1	6	9	101	102	7	1	8	13	145	138	6	1	13	18	77	77	7
1	2	5	170	172	4	1	7	9	370	370	5	1	9	13	378	388	8	1	14	18	92	98	4
1	3	5	54	48	3	1	8	9	200	200	5	1	11	13	67	66	4	1	15	18	60	57	8
1	4	5	38	35	3	1	9	9	66	69	3	1	13	13	98	100	4	1	16	18	79	80	4
1	5	5	170	171	4	1	10	9	178	175	6	1	15	13	87	85	3	1	1	19	61	69	4
1	7	5	177	164	5	1	12	9	314	312	6	1	0	14	32	30	5	1	3	19	119	130	5
1	8	5	78	79	3	1	13	9	236	227	8	1	1	14	95	95	5	1	5	19	93	91	3
1	9	5	242	233	5	1	14	9	133	132	5	1	2	14	151	150	6	1	9	19	85	87	4
1	10	5	55	52	3	1	15	9	205	212	9	1	3	14	86	82	4	1	12	19	73	74	8
1	11	5	162	163	6	1	17	9	92	89	4	1	4	14	240	244	6	1	14	19	50	52	6
1	12	5	160	163	8	1	18	9	61	63	4	1	5	14	142	137	7	1	0	20	92	95	6
1	13	5	103	105	4	1	19	9	72	59	4	1	6	14	321	325	5	1	5	20	83	90	3
1	14	5	82	82	3	1	20	9	128	120	8	1	7	14	191	186	7	1	10	20	80	75	4
1	16	5	57	62	4	1	0	10	273	257	4	1	8	14	87	92	4	1	14	20	76	75	5
1	23	5	64	60	5	1	1	10	255	243	6	1	9	14	138	144	6	1	1	21	55	51	5
1	0	6	910	932	5	1	2	10	187	180	5	1	13	14	88	91	4	1	3	21	95	97	5
1	1	6	126	126	4	1	3	10	215	206	5	1	2	15	110	103	7	1	4	21	122	122	8
1	2	6	170	171	4	1	4	10	100	97	4	1	5	15	161	156	8	1	0	22	140	141	7
1	3	6	280	287	4	1	5	10	376	366	4	1	6	15	172	178	12	1	2	22	136	139	5
1	4	6	210	214	13	1	6	10	186	185	8	1	9	15	88	94	4	1	3	22	64	60	7
1	5	6	636	638	4	1	7	10	166	169	6	1	10	15	268	276	7	1	4	22	98	101	4
1	6	6	290	298	4	1	8	10	195	191	6	1	11	15	99	102	5	1	5	22	58	59	4
1	7	6	157	146	5	1	9	10	136	134	6	1	12	15	76	74	3	1	2	23	98	93	4
1	8	6	293	282	4	1	10	10	47	51	4	1	14	15	84	83	4	1	0	24	154	150	7
1	9	6	81	81	5	1	16	10	136	135	6	1	18	15	62	54	5	1	2	24	94	96	4
1	10	6	164	161	6	1	18	10	107	113	5	1	0	16	81	81	4	1	3	25	95	87	4
1	11	6	60	68	6	1	22	10	57	50	6	1	1	16	112	118	4	1	5	25	89	78	8
1	13	6	177	183	7	1	1	11	275	253	6	1	3	16	77	78	4	2	0	0	358	374	2
1	14	6	74	76	5	1	2	11	83	85	3	1	4	16	97	97	4	2	1	0	2407	2565	15
1	16	6	71	74	3	1	5	11	131	127	9	1	5	16	146	151	10	2	2	0	1220	1251	6
1	1	7	116	118	4	1	6	11	181	179	9	1	6	16	140	143	5	2	3	0	745	745	9
1	2	7	77	84	3	1	8	11	66	66	3	1	7	16	196	192	7	2	4	0	1270	1288	10
1	3	7	289	289	4	1	10	11	73	71	3	1	9	16	67	68	4	2	5	0	384	395	3
1	4	7	94	109	6	1	11	11	111	108	5	1	10	16	156	163	12	2	6	0	1092	1089	6
1	5	7	81	78	3	1	16	11	40	34	6	1	11	16	116	112	4	2	7	0	325	325	4

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	8	0	1259	1227	4	2	2	4	143	139	4	2	8	7	83	84	3	2	3	12	219	220	9
2	9	0	149	132	5	2	3	4	882	892	8	2	9	7	241	245	5	2	4	12	79	82	5
2	10	0	96	86	13	2	4	4	98	102	4	2	10	7	70	67	3	2	5	12	65	74	3
2	11	0	379	372	5	2	5	4	121	114	4	2	11	7	140	142	5	2	6	12	179	183	6
2	12	0	130	118	12	2	6	4	60	53	2	2	13	7	234	247	6	2	7	12	231	238	6
2	13	0	222	224	7	2	8	4	143	153	5	2	14	7	124	123	6	2	8	12	89	93	3
2	14	0	296	297	6	2	9	4	105	110	5	2	23	7	119	112	5	2	9	12	329	342	11
2	16	0	167	170	6	2	10	4	433	434	5	2	23	8	83	83	6	2	10	12	114	113	5
2	1	1	78	69	4	2	11	4	171	173	6	2	1	9	415	405	4	2	12	12	50	51	4
2	2	1	534	552	3	2	12	4	148	148	8	2	2	9	233	242	8	2	13	12	86	91	3
2	3	1	629	642	6	2	13	4	171	173	6	2	3	9	558	537	4	2	2	13	103	102	4
2	4	1	48	43	2	2	15	4	189	193	7	2	4	9	236	220	6	2	4	13	179	177	6
2	5	1	85	77	3	2	16	4	177	188	6	2	5	9	152	144	7	2	5	13	69	66	3
2	6	1	260	252	4	2	1	5	119	124	4	2	6	9	79	82	3	2	6	13	107	105	4
2	7	1	442	431	4	2	2	5	411	417	6	2	7	9	276	267	5	2	7	13	159	164	7
2	9	1	45	46	3	2	3	5	133	137	6	2	9	9	96	98	5	2	8	13	113	120	7
2	10	1	106	115	4	2	4	5	229	238	4	2	10	9	88	87	6	2	9	13	243	248	6
2	11	1	91	96	4	2	5	5	374	367	4	2	11	9	182	185	7	2	10	13	66	66	3
2	12	1	350	343	5	2	6	5	727	710	6	2	12	9	341	347	10	2	11	13	267	273	6
2	21	1	95	101	5	2	7	5	667	651	4	2	15	9	98	97	4	2	17	13	62	60	4
2	0	2	1409	1456	25	2	8	5	246	255	7	2	16	9	109	109	5	2	0	14	117	120	5
2	1	2	244	253	3	2	9	5	241	225	5	2	0	10	127	137	4	2	1	14	130	129	5
2	2	2	991	1010	8	2	10	5	118	111	4	2	1	10	369	358	4	2	2	14	169	178	6
2	3	2	423	437	3	2	11	5	51	51	3	2	2	10	189	186	7	2	3	14	126	126	5
2	4	2	489	500	3	2	12	5	38	41	4	2	4	10	168	164	5	2	4	14	67	64	3
2	5	2	616	623	3	2	13	5	62	66	3	2	5	10	278	285	5	2	5	14	333	334	5
2	6	2	288	290	4	2	14	5	235	237	7	2	6	10	341	341	5	2	6	14	153	159	7
2	7	2	405	408	4	2	15	5	98	95	4	2	7	10	195	195	6	2	7	14	118	120	6
2	8	2	263	268	7	2	16	5	92	97	4	2	8	10	92	91	4	2	8	14	64	65	3
2	9	2	395	378	4	2	22	5	84	89	4	2	9	10	246	239	6	2	10	14	119	128	5
2	10	2	63	69	3	2	0	6	160	154	4	2	10	10	111	109	4	2	11	14	112	115	6
2	14	2	47	49	4	2	1	6	249	250	5	2	11	10	157	157	6	2	12	14	105	112	4
2	15	2	64	64	4	2	2	6	155	159	4	2	12	10	88	84	4	2	5	15	126	129	5
2	22	2	46	43	6	2	3	6	258	254	5	2	14	10	90	87	4	2	8	15	92	104	6
2	1	3	1484	1516	16	2	5	6	677	674	10	2	16	10	52	55	5	2	11	15	96	108	3
2	2	3	60	58	2	2	6	6	305	296	4	2	1	11	159	147	5	2	13	15	61	65	4
2	3	3	289	287	3	2	9	6	120	116	4	2	3	11	88	77	3	2	2	16	150	146	6
2	4	3	992	993	9	2	10	6	201	196	5	2	4	11	227	216	5	2	3	16	170	173	7
2	6	3	46	43	2	2	11	6	172	172	6	2	5	11	86	90	4	2	4	16	226	236	6
2	8	3	181	169	5	2	12	6	45	48	4	2	6	11	70	68	3	2	5	16	127	133	5
2	9	3	368	352	4	2	14	6	173	184	6	2	8	11	198	201	8	2	6	16	95	99	4
2	10	3	320	314	5	2	15	6	225	236	7	2	9	11	393	400	5	2	7	16	138	135	13
2	12	3	180	190	8	2	22	6	67	63	5	2	10	11	76	78	3	2	9	16	92	105	4
2	13	3	236	240	8	2	1	7	243	224	4	2	11	11	66	68	4	2	1	17	164	163	8
2	16	3	169	171	8	2	2	7	397	395	4	2	12	11	93	82	4	2	2	17	97	106	4
2	21	3	74	78	4	2	4	7	410	412	4	2	13	11	112	113	5	2	3	17	161	165	6
2	0	4	1500	1538	15	2	6	7	57	48	3	2	0	12	518	516	6	2	5	17	132	136	6
2	1	4	41	43	2	2	7	7	80	76	3	2	1	12	114	115	4	2	7	17	73	75	3

Appendix B

1,2,4-Triphenylbenzene

alues of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	8	17	114	122	4	3	1	3	713	719	11	3	5	6	364	366	4	3	13	10	99	109	3
2	9	17	63	69	4	3	2	3	325	333	3	3	7	6	60	55	5	3	1	11	165	162	6
2	10	17	114	119	5	3	3	3	665	655	8	3	8	6	137	141	5	3	3	11	113	114	8
2	14	17	67	61	7	3	4	3	171	171	6	3	10	6	97	104	4	3	4	11	84	85	4
2	17	17	73	65	5	3	5	3	109	105	4	3	11	6	144	146	9	3	5	11	137	135	6
2	0	18	113	125	6	3	6	3	401	385	7	3	13	6	53	59	4	3	6	11	96	107	5
2	1	18	62	62	4	3	7	3	463	464	6	3	15	6	85	87	3	3	8	11	54	56	5
2	3	18	85	90	6	3	8	3	67	60	3	3	22	6	102	99	4	3	9	11	284	283	9
2	7	18	78	82	4	3	9	3	62	63	3	3	23	6	46	57	7	3	11	11	182	182	7
2	8	18	75	78	6	3	10	3	143	143	5	3	1	7	619	622	7	3	13	11	221	224	8
2	9	18	132	130	5	3	11	3	63	66	4	3	3	7	224	226	6	3	14	11	122	113	5
2	10	18	58	59	5	3	13	3	123	124	5	3	4	7	536	544	8	3	15	11	73	72	4
2	1	19	174	182	7	3	15	3	98	95	4	3	5	7	163	171	6	3	0	12	162	170	6
2	2	19	79	78	4	3	21	3	46	46	7	3	7	7	162	159	6	3	2	12	160	167	7
2	4	19	126	129	6	3	0	4	850	858	7	3	9	7	254	258	12	3	5	12	186	187	6
2	6	19	63	60	4	3	1	4	259	257	4	3	10	7	51	53	4	3	6	12	126	131	6
2	13	19	75	80	4	3	2	4	282	276	4	3	11	7	182	180	6	3	7	12	83	85	3
2	3	20	75	79	5	3	3	4	233	238	6	3	14	7	72	91	3	3	9	12	126	145	9
2	12	20	48	47	6	3	4	4	84	82	4	3	15	7	117	128	7	3	11	12	261	274	6
2	13	20	78	78	4	3	5	4	84	84	3	3	20	7	58	63	6	3	12	12	126	128	4
2	3	21	68	68	4	3	6	4	759	732	4	3	21	7	88	85	4	3	13	12	204	213	7
2	6	22	63	61	6	3	7	4	57	56	4	3	23	8	61	64	6	3	14	12	70	76	4
3	1	1	501	508	6	3	9	4	144	135	5	3	1	9	464	445	4	3	15	12	96	93	4
3	2	1	643	647	6	3	10	4	96	87	4	3	2	9	207	207	5	3	1	13	53	51	4
3	3	1	45	42	2	3	11	4	149	146	8	3	3	9	53	47	4	3	2	13	75	83	5
3	4	1	616	609	4	3	12	4	122	127	5	3	4	9	143	138	5	3	3	13	176	183	6
3	5	1	108	114	4	3	13	4	124	134	5	3	5	9	189	187	6	3	5	13	398	409	10
3	6	1	82	69	3	3	14	4	50	50	4	3	6	9	107	97	4	3	7	13	141	147	7
3	7	1	507	498	11	3	15	4	187	186	12	3	7	9	40	48	5	3	8	13	152	154	7
3	8	1	552	547	4	3	21	4	115	115	4	3	8	9	86	81	3	3	9	13	94	94	4
3	9	1	116	113	4	3	1	5	851	848	13	3	9	9	171	160	8	3	10	13	72	70	3
3	11	1	140	149	6	3	2	5	69	62	5	3	10	9	58	53	4	3	11	13	87	87	4
3	12	1	58	55	5	3	3	5	609	604	4	3	11	9	127	127	6	3	16	13	91	82	5
3	13	1	261	270	6	3	5	5	348	345	4	3	12	9	101	97	3	3	1	14	65	71	4
3	14	1	400	402	6	3	6	5	30	41	4	3	13	9	141	150	6	3	2	14	255	250	6
3	15	1	339	352	6	3	7	5	183	183	7	3	15	9	83	93	5	3	5	14	80	88	5
3	0	2	1133	1165	9	3	8	5	67	60	3	3	21	9	65	65	5	3	7	14	197	201	6
3	2	2	645	645	6	3	9	5	64	61	5	3	0	10	211	200	5	3	9	14	63	58	3
3	3	2	655	660	5	3	10	5	123	119	6	3	1	10	98	94	4	3	11	14	91	91	5
3	4	2	152	154	4	3	11	5	45	40	4	3	3	10	150	149	6	3	12	14	154	157	6
3	6	2	523	513	7	3	12	5	80	75	8	3	4	10	72	65	2	3	14	14	87	87	4
3	7	2	297	304	5	3	15	5	89	97	5	3	5	10	139	132	10	3	1	15	114	109	4
3	8	2	505	478	6	3	16	5	73	79	4	3	6	10	209	206	6	3	2	15	149	154	6
3	9	2	167	179	5	3	0	6	165	180	10	3	7	10	57	51	3	3	3	15	48	50	5
3	10	2	124	132	6	3	1	6	315	303	4	3	8	10	110	105	5	3	4	15	126	120	5
3	11	2	151	150	5	3	2	6	172	180	4	3	9	10	97	97	4	3	5	15	228	229	6
3	12	2	45	39	4	3	3	6	413	408	6	3	10	10	120	118	4	3	6	15	89	85	4
3	16	2	177	182	9	3	4	6	132	123	5	3	11	10	51	50	4	3	8	15	130	130	6

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
3	9	15	114	117	5	4	1	1	87	90	5	4	13	4	218	216	7	4	20	8	67	63	5
3	10	15	87	89	4	4	2	1	268	257	4	4	14	4	284	286	9	4	22	8	65	60	5
3	11	15	90	95	4	4	5	1	247	249	4	4	15	4	174	179	7	4	1	9	308	303	5
3	19	15	74	69	6	4	6	1	37	40	3	4	16	4	128	132	6	4	2	9	50	50	3
3	2	16	193	200	6	4	7	1	101	93	5	4	20	4	117	117	5	4	3	9	53	54	5
3	3	16	165	169	8	4	8	1	208	210	7	4	21	4	56	58	5	4	7	9	64	65	3
3	5	16	101	100	5	4	10	1	170	158	6	4	22	4	113	117	6	4	8	9	146	139	6
3	6	16	190	191	7	4	11	1	58	57	3	4	1	5	107	110	4	4	9	9	213	219	7
3	11	16	125	125	8	4	13	1	144	144	7	4	2	5	207	195	4	4	10	9	210	213	7
3	12	16	42	40	5	4	14	1	50	51	4	4	3	5	67	73	5	4	11	9	107	109	4
3	1	17	78	80	8	4	0	2	703	704	6	4	4	5	116	115	5	4	13	9	102	100	3
3	3	17	56	56	5	4	1	2	406	409	4	4	5	5	378	361	5	4	14	9	51	50	5
3	5	17	56	64	5	4	2	2	58	48	3	4	6	5	78	78	3	4	0	10	348	355	5
3	9	17	64	65	4	4	3	2	68	67	3	4	7	5	355	343	4	4	2	10	274	277	5
3	12	17	90	88	4	4	4	2	53	57	4	4	8	5	102	97	5	4	3	10	253	237	6
3	13	17	60	62	4	4	5	2	536	538	4	4	10	5	159	160	6	4	5	10	61	68	6
3	0	18	64	61	4	4	6	2	205	198	5	4	11	5	100	97	4	4	10	10	208	205	8
3	2	18	98	111	7	4	8	2	116	116	5	4	12	5	108	111	6	4	11	10	229	221	7
3	4	18	71	73	4	4	9	2	102	109	5	4	14	5	117	114	5	4	12	10	252	258	7
3	5	18	110	114	4	4	10	2	227	225	6	4	16	5	190	185	9	4	15	10	60	62	5
3	7	18	66	66	4	4	11	2	164	163	7	4	0	6	385	357	4	4	18	10	81	68	4
3	8	18	58	61	5	4	12	2	137	145	5	4	1	6	386	373	7	4	2	11	140	126	5
3	2	19	86	84	5	4	13	2	107	101	7	4	2	6	596	574	11	4	4	11	168	160	6
3	8	19	90	90	4	4	16	2	62	67	4	4	3	6	80	95	3	4	5	11	396	386	6
3	0	20	90	90	5	4	1	3	394	387	6	4	4	6	230	217	5	4	7	11	75	74	3
3	2	20	90	92	4	4	2	3	115	122	6	4	5	6	167	162	5	4	8	11	100	105	4
3	3	20	107	103	4	4	3	3	155	167	5	4	6	6	84	90	4	4	9	11	71	66	4
3	4	20	78	85	4	4	4	3	180	178	5	4	8	6	97	88	4	4	10	11	71	66	3
3	12	20	80	73	4	4	5	3	524	508	6	4	9	6	179	180	6	4	11	11	145	151	5
3	2	21	108	110	4	4	6	3	110	107	6	4	10	6	72	74	3	4	16	11	72	76	4
3	4	21	68	66	5	4	7	3	413	407	5	4	11	6	156	152	7	4	0	12	175	174	6
3	13	21	64	66	5	4	8	3	67	74	3	4	15	6	56	57	4	4	1	12	355	355	5
3	4	22	90	86	4	4	9	3	432	429	7	4	23	6	68	60	5	4	2	12	157	161	6
3	5	23	57	48	5	4	10	3	270	264	6	4	1	7	210	199	6	4	3	12	115	118	8
3	10	23	69	65	5	4	12	3	226	222	6	4	2	7	95	86	6	4	5	12	171	163	6
4	0	0	779	774	4	4	14	3	75	76	4	4	3	7	293	291	4	4	6	12	205	208	6
4	1	0	140	132	5	4	15	3	189	187	8	4	4	7	145	145	5	4	9	12	193	195	8
4	3	0	191	193	4	4	16	3	54	57	5	4	5	7	245	247	6	4	10	12	205	208	11
4	4	0	216	208	4	4	0	4	172	167	4	4	6	7	281	274	5	4	11	12	163	158	6
4	5	0	109	127	8	4	1	4	139	140	5	4	8	7	142	147	9	4	12	12	149	158	7
4	6	0	200	206	5	4	2	4	494	499	5	4	9	7	146	144	6	4	13	12	104	110	4
4	7	0	50	50	3	4	3	4	156	154	7	4	10	7	233	236	6	4	16	12	65	58	4
4	8	0	123	114	5	4	4	4	192	192	5	4	11	7	77	74	3	4	1	13	58	63	3
4	9	0	585	574	6	4	5	4	146	145	5	4	12	7	65	62	5	4	2	13	166	168	6
4	13	0	87	85	3	4	6	4	309	306	4	4	13	7	136	148	5	4	3	13	271	276	7
4	14	0	110	107	5	4	8	4	62	63	4	4	16	7	95	101	4	4	4	13	248	249	6
4	15	0	166	174	7	4	10	4	63	67	3	4	19	7	102	109	4	4	7	13	121	125	9
4	16	0	143	150	6	4	11	4	200	209	9	4	20	7	67	64	5	4	8	13	139	142	5

Appendix B

1,2,4-Triphenylbenzene

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
4	9	13	68	67	3	4	3	21	49	60	5	5	2	4	324	311	7	5	12	7	54	63	4
4	10	13	108	115	4	4	6	22	50	60	6	5	3	4	122	122	5	5	14	7	63	60	4
4	11	13	164	167	6	4	1	23	61	59	5	5	4	4	208	217	9	5	15	7	132	133	5
4	0	14	214	216	6	4	4	23	51	53	6	5	5	4	226	216	6	5	1	9	139	135	5
4	2	14	333	336	7	5	1	1	123	102	8	5	6	4	134	137	5	5	2	9	102	101	5
4	3	14	219	222	8	5	2	1	95	103	5	5	7	4	131	124	5	5	3	9	89	82	3
4	4	14	185	173	7	5	3	1	212	206	4	5	8	4	106	112	5	5	4	9	248	241	7
4	5	14	94	98	4	5	4	1	215	206	5	5	14	4	163	169	6	5	5	9	76	78	3
4	7	14	74	67	6	5	6	1	340	325	5	5	15	4	95	96	4	5	6	9	89	92	3
4	8	14	161	164	9	5	7	1	69	65	3	5	20	4	79	74	4	5	7	9	82	79	4
4	10	14	163	165	5	5	8	1	240	247	5	5	1	5	143	138	7	5	9	9	130	127	5
4	12	14	71	67	4	5	9	1	103	103	6	5	2	5	190	186	6	5	10	9	82	74	6
4	1	15	109	111	6	5	10	1	288	286	5	5	3	5	211	211	5	5	11	9	114	125	5
4	2	15	191	194	7	5	11	1	135	135	8	5	4	5	337	340	4	5	12	9	118	130	6
4	3	15	125	132	8	5	12	1	243	248	7	5	5	5	216	210	7	5	13	9	115	126	8
4	4	15	193	203	7	5	13	1	99	101	4	5	6	5	140	141	5	5	0	10	57	51	3
4	5	15	61	62	4	5	14	1	94	97	3	5	7	5	221	226	5	5	2	10	181	184	6
4	6	15	117	120	5	5	15	1	87	86	6	5	8	5	70	74	3	5	5	10	97	102	4
4	7	15	100	102	5	5	16	1	102	111	10	5	9	5	92	86	4	5	6	10	146	142	9
4	8	15	55	58	4	5	22	1	47	46	7	5	10	5	106	108	4	5	10	10	124	122	4
4	9	15	156	154	6	5	23	1	68	62	5	5	11	5	187	189	8	5	11	10	158	160	6
4	13	15	60	60	5	5	0	2	854	833	11	5	12	5	93	97	3	5	13	10	57	55	4
4	1	16	109	114	4	5	1	2	191	197	5	5	13	5	117	121	6	5	14	10	83	85	3
4	2	16	66	65	3	5	2	2	397	402	5	5	15	5	261	269	7	5	16	10	85	85	3
4	3	16	212	222	7	5	3	2	166	156	7	5	0	6	445	433	10	5	17	10	98	97	4
4	4	16	61	64	3	5	4	2	196	203	5	5	1	6	55	56	4	5	1	11	224	232	8
4	5	16	110	113	5	5	5	2	80	85	3	5	3	6	551	555	9	5	3	11	383	379	5
4	6	16	136	137	5	5	6	2	121	111	4	5	4	6	268	262	5	5	4	11	332	330	5
4	9	16	85	81	4	5	7	2	56	57	4	5	5	6	62	64	3	5	5	11	418	415	5
4	10	16	70	71	4	5	9	2	171	167	7	5	6	6	46	49	3	5	6	11	157	156	5
4	13	16	61	56	4	5	10	2	276	282	6	5	7	6	103	100	4	5	7	11	220	213	6
4	1	17	64	65	4	5	11	2	208	211	6	5	9	6	230	238	9	5	8	11	132	129	5
4	5	17	74	72	4	5	14	2	213	220	7	5	10	6	71	70	5	5	9	11	80	82	5
4	8	17	56	53	4	5	15	2	108	117	5	5	11	6	222	224	6	5	11	11	87	89	5
4	9	17	103	103	5	5	1	3	714	700	6	5	14	6	151	157	6	5	13	11	65	63	4
4	10	17	88	82	5	5	2	3	589	581	4	5	16	6	105	108	5	5	17	11	97	92	5
4	13	17	89	86	4	5	3	3	299	288	9	5	21	6	76	74	4	5	1	12	183	182	8
4	0	18	44	52	5	5	4	3	379	386	6	5	1	7	309	310	7	5	3	12	207	215	7
4	3	18	117	118	5	5	5	3	52	43	3	5	2	7	211	215	5	5	4	12	266	275	8
4	5	18	167	166	7	5	6	3	116	123	6	5	3	7	332	336	10	5	5	12	329	336	6
4	8	18	74	71	5	5	7	3	140	138	7	5	4	7	85	91	4	5	6	12	54	55	7
4	2	19	72	74	4	5	8	3	175	169	6	5	5	7	68	63	3	5	7	12	68	67	3
4	3	19	70	79	7	5	9	3	77	75	3	5	6	7	123	125	4	5	8	12	71	69	4
4	14	19	67	65	5	5	10	3	122	123	8	5	7	7	109	107	4	5	10	12	41	34	5
4	0	20	79	83	3	5	11	3	326	330	6	5	8	7	159	157	6	5	12	12	109	112	4
4	4	20	63	70	6	5	13	3	88	87	4	5	9	7	48	56	4	5	14	12	70	78	4
4	6	20	61	59	4	5	14	3	100	93	7	5	10	7	123	130	4	5	20	12	74	68	5
4	12	20	86	86	4	5	15	3	65	68	4	5	11	7	171	178	7	5	1	13	298	307	6

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
5	2	13	70	69	3	6	6	0	49	52	3	6	4	4	90	91	4	6	7	9	96	97	4
5	3	13	111	114	6	6	7	0	194	199	10	6	5	4	56	57	3	6	9	9	120	117	4
5	4	13	217	225	7	6	8	0	90	89	3	6	8	4	52	54	4	6	10	9	53	58	8
5	11	13	114	112	4	6	9	0	160	161	12	6	9	4	129	134	6	6	11	9	157	159	6
5	12	13	80	81	4	6	10	0	127	126	5	6	12	4	87	88	3	6	12	9	92	92	4
5	13	13	87	89	4	6	12	0	110	113	5	6	13	4	137	145	6	6	16	9	121	121	4
5	15	13	105	106	8	6	13	0	212	210	7	6	16	4	47	53	5	6	0	10	207	202	6
5	0	14	90	88	4	6	14	0	170	162	8	6	1	5	91	84	4	6	2	10	189	175	6
5	4	14	80	81	5	6	16	0	95	101	4	6	2	5	76	78	3	6	5	10	137	130	5
5	5	14	66	64	3	6	1	1	266	255	6	6	3	5	62	51	4	6	7	10	39	44	5
5	9	14	63	61	4	6	2	1	93	91	4	6	6	5	96	98	4	6	8	10	79	73	4
5	10	14	111	117	8	6	3	1	43	37	3	6	7	5	125	126	5	6	9	10	87	94	4
5	14	14	66	68	4	6	4	1	91	98	5	6	8	5	79	81	3	6	12	10	109	111	5
5	15	14	70	70	4	6	5	1	279	295	7	6	10	5	287	291	8	6	13	10	102	104	3
5	19	14	98	87	5	6	6	1	64	60	3	6	11	5	73	74	3	6	15	10	76	75	4
5	1	15	122	127	5	6	7	1	57	57	5	6	12	5	159	160	6	6	1	11	188	192	6
5	6	15	178	176	9	6	8	1	93	96	4	6	14	5	181	195	7	6	2	11	264	268	6
5	7	15	129	132	7	6	10	1	185	187	7	6	16	5	104	113	6	6	4	11	314	306	6
5	8	15	61	67	4	6	12	1	153	150	9	6	0	6	203	192	5	6	6	11	110	105	4
5	10	15	74	75	5	6	13	1	140	140	5	6	2	6	63	66	3	6	7	11	143	150	6
5	12	15	82	79	4	6	14	1	101	104	4	6	3	6	301	297	8	6	8	11	75	76	5
5	18	15	100	90	5	6	16	1	44	39	6	6	4	6	146	142	7	6	20	11	98	83	6
5	0	16	50	52	4	6	1	2	157	158	5	6	5	6	55	52	7	6	0	12	209	203	6
5	3	16	121	132	5	6	2	2	226	234	5	6	6	6	163	163	6	6	1	12	128	132	5
5	4	16	74	77	3	6	3	2	277	281	9	6	8	6	157	163	6	6	3	12	136	144	6
5	5	16	68	72	4	6	4	2	246	248	7	6	9	6	104	102	6	6	4	12	72	72	4
5	11	16	61	68	4	6	5	2	108	108	5	6	10	6	198	205	7	6	6	12	105	108	5
5	12	16	103	100	8	6	6	2	158	161	6	6	14	6	179	188	7	6	8	12	193	198	7
5	13	16	48	52	7	6	8	2	76	79	4	6	18	6	98	105	5	6	11	12	98	104	5
5	17	16	45	30	7	6	9	2	285	288	6	6	19	6	93	91	4	6	17	12	55	52	6
5	6	17	79	82	4	6	11	2	90	90	4	6	1	7	54	55	3	6	18	12	88	75	5
5	10	17	88	80	4	6	12	2	133	136	5	6	2	7	88	96	4	6	19	12	84	73	7
5	12	17	78	77	4	6	14	2	87	90	3	6	3	7	52	57	3	6	1	13	154	160	8
5	4	18	97	101	4	6	22	2	75	71	8	6	4	7	148	159	8	6	2	13	227	229	7
5	2	19	59	61	4	6	1	3	349	350	5	6	5	7	49	47	5	6	3	13	204	201	7
5	8	19	57	63	7	6	2	3	89	80	6	6	6	7	165	171	6	6	4	13	103	103	4
5	10	19	94	88	4	6	4	3	165	163	6	6	7	7	232	236	8	6	8	13	64	68	4
5	4	20	42	39	6	6	5	3	79	75	4	6	8	7	108	110	4	6	11	13	53	57	5
5	7	20	65	63	4	6	7	3	293	296	8	6	10	7	102	106	3	6	19	13	95	77	5
5	11	20	67	57	5	6	8	3	72	77	4	6	11	7	114	113	4	6	0	14	93	97	3
5	5	22	71	68	7	6	9	3	175	172	7	6	12	7	187	197	7	6	2	14	147	151	6
5	7	22	88	83	4	6	10	3	205	196	8	6	14	7	137	141	6	6	3	14	134	133	5
6	0	0	523	514	6	6	11	3	202	203	7	6	15	7	96	92	6	6	4	14	257	261	7
6	1	0	241	226	5	6	12	3	70	73	4	6	18	7	72	74	4	6	6	14	80	82	4
6	2	0	324	319	5	6	14	3	87	89	7	6	21	7	58	58	6	6	7	14	65	64	4
6	3	0	155	151	5	6	21	3	88	82	9	6	3	9	115	109	5	6	8	14	71	74	4
6	4	0	112	101	8	6	0	4	284	293	5	6	4	9	63	65	3	6	13	14	51	48	5
6	5	0	171	173	6	6	3	4	328	337	5	6	5	9	119	122	4	6	2	15	57	66	8

Appendix B

1,2,4-Triphenylbenzene

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
6	4	15	130	131	5	7	15	2	52	53	6	7	15	7	71	75	6	7	2	15	178	178	7
6	7	15	70	68	4	7	16	2	96	97	4	7	16	8	61	68	5	7	3	15	74	73	4
6	8	15	76	73	4	7	22	2	53	50	6	7	3	9	57	57	4	7	4	15	56	60	5
6	11	15	69	70	4	7	1	3	67	66	3	7	4	9	318	302	8	7	5	15	115	115	4
6	1	16	73	72	4	7	2	3	54	53	4	7	5	9	208	211	7	7	10	15	91	85	4
6	2	16	143	140	6	7	4	3	104	98	4	7	6	9	83	85	4	7	12	15	67	66	5
6	4	16	83	87	4	7	5	3	167	172	6	7	7	9	83	81	4	7	13	15	56	53	5
6	7	16	70	70	4	7	7	3	483	485	11	7	8	9	66	60	4	7	16	15	62	54	5
6	10	16	103	107	4	7	8	3	266	271	6	7	9	9	119	114	4	7	0	16	55	51	4
6	11	16	61	65	6	7	10	3	232	229	8	7	11	9	49	47	5	7	2	16	95	107	4
6	1	17	59	63	4	7	11	3	161	163	9	7	12	9	68	66	4	7	3	16	106	106	6
6	3	17	41	47	6	7	12	3	160	163	6	7	0	10	239	237	10	7	4	16	88	91	4
6	4	17	56	63	5	7	0	4	160	153	6	7	1	10	95	90	4	7	5	16	126	128	5
6	5	17	67	62	4	7	2	4	156	146	7	7	2	10	63	60	4	7	10	16	49	45	5
6	9	17	62	64	4	7	4	4	41	45	4	7	3	10	72	78	4	7	9	17	70	63	5
6	11	17	140	142	8	7	6	4	260	255	6	7	4	10	170	169	11	7	10	17	82	78	5
6	13	17	87	80	4	7	7	4	102	106	3	7	5	10	95	92	4	7	12	17	123	111	5
6	6	18	130	138	5	7	8	4	115	111	5	7	6	10	71	69	4	7	0	18	68	61	4
6	6	19	69	75	8	7	9	4	94	96	5	7	11	10	123	126	6	7	4	18	83	89	4
6	8	19	89	87	4	7	10	4	213	210	7	7	13	10	62	66	4	7	2	19	57	52	5
6	10	19	77	72	4	7	15	4	101	109	6	7	1	11	138	132	5	7	3	19	68	69	4
6	11	19	76	76	5	7	2	5	140	137	5	7	2	11	278	278	6	7	6	19	89	91	6
6	5	20	65	63	4	7	3	5	250	258	6	7	3	11	98	93	5	7	0	20	71	67	8
6	10	20	83	83	5	7	4	5	53	53	4	7	4	11	125	135	5	7	2	20	70	63	5
6	2	23	47	44	6	7	5	5	82	86	4	7	5	11	109	111	4	7	1	21	59	55	6
7	1	1	186	172	10	7	6	5	184	189	7	7	7	11	130	132	5	7	2	21	61	55	5
7	2	1	151	147	7	7	8	5	238	239	6	7	9	11	69	75	4	7	4	22	75	66	5
7	3	1	179	179	10	7	10	5	88	82	4	7	10	11	82	86	4	8	0	0	57	60	6
7	4	1	50	53	4	7	12	5	72	73	4	7	11	11	86	78	4	8	2	0	118	129	5
7	5	1	122	117	7	7	0	6	101	106	4	7	13	11	83	84	4	8	3	0	154	153	6
7	6	1	99	100	3	7	2	6	169	165	6	7	15	11	81	78	4	8	4	0	104	103	4
7	7	1	105	111	4	7	3	6	167	172	8	7	3	12	226	243	7	8	5	0	103	100	4
7	9	1	53	51	4	7	4	6	92	88	4	7	4	12	79	86	4	8	6	0	252	255	7
7	11	1	88	93	4	7	5	6	204	209	6	7	5	12	105	101	5	8	7	0	318	327	9
7	12	1	145	149	6	7	6	6	221	228	9	7	6	12	66	72	4	8	8	0	416	426	6
7	13	1	142	140	5	7	7	6	161	161	6	7	8	12	61	61	5	8	9	0	336	331	7
7	14	1	67	63	4	7	8	6	129	128	7	7	18	12	92	86	4	8	10	0	114	121	5
7	20	1	63	65	6	7	10	6	140	152	6	7	2	13	194	195	7	8	11	0	73	72	4
7	0	2	58	53	5	7	13	6	93	103	4	7	3	13	169	159	6	8	12	0	182	187	8
7	1	2	243	234	5	7	14	6	98	98	5	7	4	13	58	70	5	8	13	0	67	69	4
7	2	2	137	136	5	7	17	6	85	89	5	7	6	13	64	59	5	8	14	0	56	57	7
7	4	2	64	65	3	7	2	7	90	95	7	7	7	13	113	112	4	8	1	1	225	220	6
7	6	2	203	200	11	7	5	7	53	49	4	7	1	14	169	171	7	8	2	1	52	58	4
7	8	2	320	327	6	7	6	7	152	163	10	7	2	14	98	97	5	8	3	1	188	199	8
7	11	2	349	355	7	7	7	7	70	76	4	7	4	14	112	109	4	8	4	1	264	261	6
7	12	2	61	63	4	7	9	7	137	134	5	7	5	14	82	78	4	8	6	1	164	158	6
7	13	2	49	59	5	7	11	7	175	180	9	7	6	14	71	66	4	8	7	1	196	185	7
7	14	2	85	86	5	7	12	7	60	66	4	7	9	14	82	84	5	8	10	1	175	168	7

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
8	14	1	58	61	6	8	7	7	99	101	4	9	3	2	87	85	4	9	13	9	94	96	4
8	15	1	56	63	6	8	11	7	48	53	5	9	4	2	114	115	4	9	1	10	133	136	6
8	0	2	68	67	4	8	19	7	62	55	6	9	5	2	159	165	9	9	3	10	71	70	4
8	2	2	72	68	3	8	1	9	78	78	3	9	6	2	100	99	3	9	5	10	65	60	4
8	3	2	140	142	6	8	3	9	109	125	7	9	9	2	172	172	7	9	8	10	87	89	4
8	4	2	208	215	7	8	8	9	67	65	4	9	12	2	54	57	5	9	9	10	66	64	5
8	5	2	166	165	9	8	9	9	95	95	5	9	13	2	85	85	4	9	11	10	46	50	6
8	7	2	122	114	7	8	10	9	81	85	4	9	14	2	75	76	5	9	16	10	84	73	5
8	8	2	169	169	8	8	11	9	58	60	5	9	17	2	72	73	4	9	1	11	91	94	4
8	9	2	185	183	7	8	12	9	116	120	6	9	1	3	152	148	8	9	3	11	89	86	4
8	10	2	66	65	4	8	13	9	74	75	4	9	2	3	103	105	4	9	5	11	56	50	5
8	13	2	84	84	4	8	0	10	225	220	7	9	3	3	88	89	4	9	14	11	53	46	6
8	15	2	65	65	6	8	1	10	87	84	3	9	4	3	105	109	4	9	0	12	53	52	8
8	17	2	48	48	6	8	2	10	64	59	4	9	6	3	69	68	3	9	4	12	61	68	5
8	1	3	121	120	5	8	3	10	95	86	3	9	7	3	108	108	10	9	5	12	80	87	5
8	4	3	45	42	5	8	12	10	90	91	5	9	8	3	44	40	5	9	11	12	86	87	5
8	5	3	219	226	6	8	4	11	108	106	4	9	9	3	115	117	4	9	3	13	75	76	4
8	6	3	102	103	4	8	5	11	111	109	4	9	13	3	87	86	6	9	11	14	78	71	5
8	7	3	333	335	6	8	7	11	89	91	4	9	15	3	84	81	7	9	13	14	61	50	5
8	18	3	58	55	5	8	8	11	58	59	5	9	0	4	123	127	5	9	2	15	50	51	5
8	0	4	68	75	3	8	12	11	87	85	4	9	3	4	36	39	5	9	3	15	62	63	4
8	1	4	111	108	5	8	13	11	74	70	5	9	6	4	125	134	5	9	4	15	50	51	5
8	2	4	284	279	7	8	0	12	172	180	6	9	7	4	122	129	5	9	9	15	57	57	5
8	3	4	85	87	3	8	5	12	83	87	3	9	9	4	80	77	4	9	10	15	56	48	6
8	5	4	269	285	6	8	11	12	122	117	4	9	11	4	97	100	3	9	2	16	61	56	5
8	6	4	80	82	3	8	13	12	94	89	8	9	13	4	55	54	6	9	3	16	73	73	4
8	7	4	95	96	4	8	3	13	109	109	5	9	15	4	66	70	4	9	6	16	64	61	5
8	8	4	106	106	4	8	6	13	77	82	6	9	3	5	73	71	4	9	1	17	60	49	5
8	11	4	105	110	5	8	11	13	66	54	4	9	5	5	155	162	5	9	10	17	56	44	8
8	1	5	214	223	6	8	3	14	130	130	5	9	11	5	129	128	7	9	1	18	81	79	5
8	2	5	69	72	3	8	4	14	48	41	7	9	2	6	152	146	6	9	3	18	110	105	4
8	3	5	64	69	4	8	2	15	100	104	4	9	3	6	96	97	4	9	8	18	55	52	6
8	5	5	153	155	6	8	8	15	54	55	5	9	5	6	201	215	7	9	3	19	81	82	4
8	6	5	212	219	7	8	1	16	57	58	5	9	11	6	91	91	3	9	5	19	107	102	5
8	7	5	62	63	4	8	2	16	178	176	7	9	1	7	175	174	6	10	0	0	244	239	12
8	0	6	145	144	8	8	3	16	122	128	5	9	2	7	68	73	5	10	2	0	229	222	10
8	3	6	85	91	3	8	4	16	85	81	4	9	3	7	54	53	5	10	3	0	82	88	5
8	5	6	112	119	5	8	4	18	70	70	4	9	5	7	86	90	4	10	4	0	107	112	5
8	6	6	91	95	4	8	5	18	60	58	5	9	8	7	74	70	3	10	5	0	116	118	4
8	8	6	68	75	4	8	0	20	67	57	5	9	9	7	59	62	6	10	6	0	98	106	6
8	9	6	59	60	5	8	1	20	48	52	7	9	12	7	67	69	4	10	9	0	151	158	6
8	10	6	201	210	7	9	2	1	147	159	6	9	17	7	73	65	5	10	11	0	105	98	4
8	16	6	62	60	5	9	5	1	193	192	9	9	16	8	102	98	4	10	12	0	47	46	6
8	1	7	62	67	3	9	7	1	314	317	8	9	1	9	169	175	8	10	2	1	87	81	4
8	2	7	108	108	4	9	9	1	151	156	6	9	2	9	90	85	4	10	3	1	121	121	6
8	3	7	104	104	3	9	10	1	78	74	4	9	5	9	115	116	4	10	4	1	160	161	10
8	4	7	96	102	4	9	0	2	106	102	5	9	9	9	58	61	5	10	6	1	121	125	8
8	5	7	113	110	4	9	1	2	55	58	4	9	12	9	112	100	6	10	9	1	126	120	7

Appendix B

1,2,4-Triphenylbenzene

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
10	0	2	207	204	8	11	4	1	73	74	4	12	9	7	67	65	5						
10	2	2	101	100	5	11	5	1	61	65	4	12	0	10	63	60	5						
10	3	2	80	89	4	11	6	1	65	65	5	13	1	1	70	79	6						
10	5	2	65	63	4	11	7	1	143	143	9	13	6	1	49	52	6						
10	7	2	213	213	8	11	8	1	70	67	4	13	5	2	49	54	6						
10	9	2	86	81	4	11	9	1	81	80	4	13	9	2	50	46	6						
10	10	2	100	101	4	11	0	2	66	75	4	13	3	3	56	55	6						
10	15	2	56	52	7	11	1	2	53	52	5	13	6	3	46	41	6						
10	1	3	71	72	4	11	3	2	64	55	6	13	8	3	71	82	5						
10	5	3	83	80	3	11	4	2	84	83	5	13	7	5	99	93	4						
10	7	3	98	105	9	11	6	2	125	119	6	13	8	5	80	81	5						
10	9	3	138	139	5	11	8	2	126	127	6	13	7	6	53	61	8						
10	0	4	66	73	4	11	9	2	63	68	5	13	4	9	82	75	7						
10	3	4	63	66	5	11	1	3	79	83	4	13	3	11	63	57	6						
10	4	4	101	110	6	11	5	3	55	58	5	13	4	11	70	59	7						
10	7	4	207	200	11	11	6	3	56	64	5												
10	9	4	86	86	4	11	9	3	51	53	6												
10	11	4	71	69	5	11	7	4	94	101	5												
10	1	5	126	131	5	11	13	4	60	58	6												
10	3	5	54	68	4	11	2	5	69	70	4												
10	5	5	107	111	5	11	5	5	49	55	6												
10	7	5	147	149	6	11	8	5	92	89	4												
10	14	5	65	62	5	11	10	5	95	95	4												
10	5	6	116	122	9	11	3	6	45	43	5												
10	6	6	49	50	5	11	2	7	50	51	6												
10	7	6	61	66	5	11	4	7	74	72	4												
10	9	6	48	51	5	11	6	7	70	69	4												
10	1	7	148	154	8	11	8	7	92	89	4												
10	6	7	106	108	4	11	6	8	79	78	5												
10	11	7	42	41	6	11	2	9	74	63	5												
10	12	7	44	42	6	11	0	10	66	72	5												
10	17	7	55	50	7	11	2	11	104	105	5												
10	11	8	90	87	4	11	3	11	72	76	4												
10	3	9	56	52	7	11	4	11	75	69	5												
10	4	9	94	95	6	11	4	14	48	40	7												
10	12	9	83	82	4	11	6	14	59	52	6												
10	0	10	110	106	5	11	0	16	52	46	6												
10	1	10	75	72	4	12	0	0	108	122	5												
10	3	10	61	69	7	12	9	1	51	46	5												
10	13	10	108	100	6	12	1	2	47	53	6												
10	8	11	50	47	6	12	4	2	52	52	6												
10	10	12	50	48	6	12	7	2	70	73	5												
10	2	13	54	58	6	12	1	3	75	74	4												
10	5	14	77	72	4	12	8	4	114	114	9												
10	5	15	58	60	6	12	10	4	78	83	7												
10	4	16	60	54	6	12	5	5	71	73	4												
10	6	16	67	63	6	12	3	6	59	58	5												
11	1	1	189	188	9	12	8	6	76	79	5												

Appendix B

$2^2,4^5$-Diphenyl-p-quinquephenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
0	2	0	351	378	2	0	12	2	293	281	6	0	3	5	76	79	3	1	6	-5	85	89	3
0	4	0	340	379	3	0	15	2	71	64	3	0	6	5	63	59	4	1	7	-5	98	100	4
0	6	0	202	208	5	0	17	2	187	184	6	0	7	5	69	71	3	1	8	-5	160	153	6
0	8	0	110	97	5	0	18	2	151	147	7	0	9	5	243	241	9	1	9	-5	63	72	4
0	10	0	172	176	6	0	20	2	55	52	4	0	11	5	50	57	5	1	10	-5	68	67	4
0	12	0	162	153	5	0	26	2	62	66	4	0	14	5	232	231	8	1	11	-5	39	39	6
0	14	0	622	595	6	0	29	2	64	61	4	0	16	5	78	77	4	1	12	-5	135	138	5
0	16	0	788	748	6	0	1	3	85	91	4	0	17	5	43	42	6	1	14	-5	147	151	7
0	18	0	68	72	3	0	2	3	102	96	4	0	21	5	179	175	7	1	16	-5	117	124	5
0	24	0	45	44	5	0	3	3	310	324	6	0	23	5	161	160	7	1	19	-5	134	126	4
0	26	0	48	47	5	0	4	3	66	67	3	0	25	5	74	74	4	1	20	-5	134	126	5
0	28	0	46	52	5	0	6	3	315	334	6	0	27	5	68	73	5	1	21	-5	79	86	5
0	30	0	184	195	7	0	7	3	353	374	6	0	28	5	84	74	5	1	23	-5	61	68	5
0	32	0	102	106	5	0	10	3	34	32	4	0	30	5	78	70	5	1	24	-5	61	62	5
0	1	1	97	103	5	0	11	3	48	49	3	0	0	6	45	42	5	1	26	-5	78	67	6
0	2	1	535	587	4	0	12	3	195	186	7	0	1	6	48	49	5	1	27	-5	60	59	5
0	3	1	306	337	4	0	13	3	136	136	6	0	3	6	93	98	3	1	30	-5	72	55	5
0	4	1	238	257	4	0	15	3	143	149	5	0	5	6	43	43	5	1	0	-4	160	163	7
0	5	1	965	1058	4	0	16	3	42	41	4	0	6	6	93	89	5	1	2	-4	276	276	7
0	6	1	837	908	4	0	17	3	70	62	3	0	7	6	62	61	4	1	3	-4	210	212	7
0	7	1	166	190	6	0	20	3	70	71	4	0	9	6	78	77	4	1	4	-4	136	140	5
0	8	1	228	240	6	0	21	3	87	84	4	0	11	6	77	76	4	1	5	-4	71	68	3
0	9	1	119	128	4	0	22	3	103	108	4	0	17	6	104	101	4	1	6	-4	193	188	6
0	10	1	132	151	6	0	23	3	105	104	5	0	19	6	56	63	5	1	7	-4	108	123	4
0	11	1	274	272	6	0	24	3	46	42	5	0	8	7	135	132	5	1	10	-4	82	84	3
0	12	1	179	182	6	0	26	3	178	173	8	0	12	7	101	104	4	1	11	-4	181	193	7
0	13	1	79	82	2	0	0	4	44	40	4	0	3	8	84	79	5	1	12	-4	46	50	4
0	14	1	228	225	7	0	1	4	218	236	7	0	4	8	78	74	6	1	13	-4	69	73	3
0	16	1	197	174	7	0	3	4	35	33	4	0	7	8	103	104	6	1	14	-4	170	165	6
0	19	1	179	167	7	0	4	4	253	260	7	0	9	8	71	66	5	1	15	-4	109	106	4
0	20	1	145	142	6	0	5	4	40	35	4	1	3	-7	53	55	5	1	16	-4	82	80	4
0	21	1	108	107	4	0	6	4	168	174	6	1	9	-7	72	71	4	1	20	-4	43	44	5
0	24	1	60	62	4	0	7	4	164	163	6	1	14	-7	82	84	5	1	23	-4	51	46	5
0	27	1	72	76	4	0	8	4	75	77	4	1	16	-7	78	79	5	1	25	-4	103	105	5
0	32	1	54	58	5	0	9	4	37	36	4	1	0	-6	54	51	4	1	26	-4	49	58	6
0	36	1	54	59	7	0	11	4	194	199	7	1	2	-6	70	71	4	1	27	-4	87	87	6
0	0	2	436	483	5	0	14	4	137	146	7	1	13	-6	117	116	4	1	28	-4	90	87	6
0	1	2	1000	1106	5	0	17	4	103	99	3	1	14	-6	81	83	5	1	29	-4	100	101	5
0	2	2	632	667	5	0	18	4	137	144	6	1	16	-6	43	33	6	1	1	-3	165	171	6
0	3	2	147	161	5	0	20	4	78	79	4	1	18	-6	81	84	4	1	2	-3	146	138	5
0	4	2	348	378	5	0	21	4	117	115	5	1	19	-6	102	105	4	1	3	-3	104	106	5
0	5	2	164	188	6	0	22	4	51	52	5	1	20	-6	54	55	5	1	4	-3	383	388	6
0	6	2	562	592	5	0	24	4	47	49	5	1	27	-6	60	61	6	1	5	-3	347	345	6
0	7	2	172	180	6	0	25	4	78	79	5	1	1	-5	95	92	4	1	6	-3	332	341	6
0	8	2	113	111	4	0	26	4	73	82	5	1	2	-5	51	48	4	1	7	-3	311	314	6
0	9	2	110	110	4	0	27	4	110	99	5	1	3	-5	145	133	6	1	8	-3	52	52	3
0	10	2	195	195	6	0	1	5	46	39	4	1	4	-5	102	103	4	1	9	-3	379	375	6
0	11	2	138	135	5	0	2	5	56	54	4	1	5	-5	112	112	4	1	11	-3	170	168	6

Appendix B

$2^2,4^5$-Diphenyl-p-quinquephenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF
1	12	-3	293	295	7
1	13	-3	246	247	7
1	15	-3	88	82	5
1	17	-3	109	96	3
1	19	-3	53	51	4
1	20	-3	90	87	4
1	23	-3	71	72	4
1	24	-3	76	70	4
1	28	-3	51	58	5
1	29	-3	93	92	4
1	30	-3	44	43	6
1	0	-2	1663	1750	5
1	1	-2	49	41	4
1	2	-2	1191	1262	5
1	4	-2	181	185	6
1	5	-2	162	173	6
1	6	-2	234	241	6
1	7	-2	641	658	5
1	8	-2	105	111	5
1	9	-2	335	333	6
1	10	-2	251	249	6
1	12	-2	237	241	7
1	13	-2	115	130	4
1	14	-2	492	459	6
1	16	-2	314	300	7
1	18	-2	135	125	6
1	22	-2	71	72	4
1	23	-2	65	64	4
1	24	-2	114	109	5
1	26	-2	78	84	4
1	27	-2	52	44	5
1	28	-2	49	57	5
1	30	-2	181	190	8
1	1	-1	472	468	4
1	2	-1	555	549	4
1	3	-1	1256	1299	4
1	4	-1	313	327	5
1	5	-1	472	480	5
1	6	-1	339	343	5
1	7	-1	80	83	3
1	8	-1	261	275	5
1	9	-1	66	72	3
1	11	-1	167	154	6
1	12	-1	95	101	4
1	13	-1	351	354	6
1	14	-1	139	149	6
1	15	-1	286	277	7
1	16	-1	82	77	3
1	17	-1	64	67	4
1	19	-1	209	209	7
1	20	-1	227	211	8
1	21	-1	45	67	6
1	23	-1	72	68	3
1	25	-1	79	80	4
1	28	-1	166	167	6
1	0	0	466	442	4
1	1	0	348	340	4
1	2	0	209	192	4
1	3	0	215	213	4
1	4	0	182	177	5
1	5	0	311	316	4
1	6	0	220	231	5
1	7	0	112	122	5
1	8	0	153	155	6
1	9	0	211	219	6
1	12	0	118	112	5
1	14	0	119	109	5
1	15	0	38	49	5
1	17	0	84	77	3
1	20	0	80	80	3
1	24	0	84	91	4
1	26	0	86	80	3
1	28	0	52	51	5
1	32	0	58	58	6
1	1	1	370	380	5
1	2	1	565	575	5
1	3	1	302	305	5
1	4	1	396	418	5
1	5	1	280	289	5
1	6	1	160	161	6
1	7	1	179	188	6
1	8	1	103	112	4
1	9	1	146	140	6
1	12	1	61	64	3
1	14	1	290	282	7
1	15	1	125	133	4
1	16	1	140	133	5
1	18	1	90	94	3
1	19	1	157	160	6
1	21	1	179	167	7
1	25	1	89	84	4
1	27	1	50	59	6
1	0	2	621	640	5
1	1	2	205	208	6
1	2	2	501	515	5
1	3	2	82	86	3
1	4	2	106	99	4
1	5	2	312	307	6
1	6	2	75	77	3
1	7	2	49	55	3
1	8	2	61	62	3
1	10	2	144	142	6
1	11	2	116	105	5
1	12	2	68	71	3
1	15	2	135	138	5
1	18	2	150	150	6
1	20	2	87	92	4
1	21	2	163	159	7
1	24	2	70	71	4
1	26	2	121	126	4
1	27	2	165	163	6
1	28	2	122	126	5
1	30	2	47	36	6
1	1	3	73	66	2
1	2	3	192	201	7
1	3	3	60	58	3
1	4	3	328	326	7
1	6	3	123	132	4
1	7	3	631	621	7
1	8	3	104	105	4
1	9	3	183	175	6
1	10	3	46	47	4
1	11	3	163	156	6
1	13	3	89	85	4
1	14	3	81	89	4
1	16	3	264	258	8
1	18	3	37	34	6
1	20	3	146	141	6
1	21	3	358	340	9
1	22	3	94	108	4
1	23	3	379	365	9
1	25	3	146	139	6
1	30	3	67	63	5
1	0	4	108	103	3
1	1	4	357	366	7
1	4	4	55	53	4
1	5	4	97	86	4
1	6	4	254	254	7
1	8	4	76	76	3
1	9	4	69	71	4
1	10	4	59	57	4
1	11	4	162	171	7
1	12	4	79	78	5
1	13	4	72	65	4
1	14	4	78	80	3
1	16	4	107	110	6
1	17	4	133	135	6
1	18	4	106	98	4
1	19	4	179	178	7
1	21	4	121	120	5
1	24	4	70	69	4
1	25	4	58	62	5
1	27	4	93	89	4
1	2	5	174	183	7
1	4	5	59	61	4
1	5	5	127	132	4
1	6	5	160	162	7
1	8	5	63	65	4
1	9	5	75	72	4
1	10	5	124	124	5
1	11	5	49	50	6
1	12	5	114	110	4
1	13	5	77	75	4
1	14	5	47	57	6
1	17	5	84	85	4
1	19	5	65	66	4
1	20	5	108	111	5
1	21	5	112	114	6
1	0	6	129	134	4
1	3	6	127	125	4
1	4	6	111	117	5
1	5	6	119	122	4
1	7	6	157	159	6
1	9	6	56	54	5
1	11	6	71	73	4
1	15	6	84	85	4
1	16	6	64	65	5
1	17	6	60	62	6
1	18	6	63	54	5
1	4	7	89	92	4
1	5	7	68	67	5
1	8	7	57	64	5
1	9	7	68	72	6
1	12	7	47	53	7
1	7	8	68	71	5
2	1	-7	88	82	4
2	2	-7	44	39	6
2	3	-7	80	84	4
2	4	-7	68	63	4
2	5	-7	53	53	5
2	6	-7	78	81	5
2	14	-7	120	113	4

Appendix B

$2^{2},4^{5}$-Diphenyl-p-quinquephenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	15	-7	53	57	6	2	5	-3	383	380	6	2	23	-1	67	83	5	2	5	2	241	220	7
2	16	-7	119	124	5	2	6	-3	324	309	6	2	25	-1	73	96	5	2	6	2	67	66	3
2	19	-7	53	54	6	2	7	-3	165	167	6	2	27	-1	92	95	4	2	9	2	110	107	6
2	20	-7	72	70	5	2	8	-3	110	109	5	2	29	-1	74	74	4	2	10	2	69	63	3
2	21	-7	79	83	5	2	9	-3	265	270	7	2	30	-1	77	87	5	2	11	2	138	134	5
2	23	-7	44	29	6	2	11	-3	125	115	5	2	35	-1	48	46	7	2	12	2	232	216	7
2	0	-6	237	234	9	2	12	-3	87	82	3	2	1	0	241	238	6	2	13	2	173	164	6
2	1	-6	99	94	5	2	13	-3	70	73	3	2	2	0	156	149	6	2	18	2	201	204	8
2	2	-6	94	94	4	2	14	-3	55	56	4	2	3	0	189	174	6	2	19	2	258	249	8
2	3	-6	55	50	4	2	16	-3	65	68	4	2	4	0	134	126	6	2	20	2	117	112	3
2	5	-6	77	76	4	2	19	-3	142	145	6	2	5	0	67	69	2	2	21	2	253	243	9
2	11	-6	93	94	4	2	22	-3	97	90	4	2	7	0	113	99	4	2	22	2	51	53	6
2	15	-6	147	147	6	2	24	-3	81	74	4	2	9	0	117	112	4	2	23	2	129	128	5
2	16	-6	151	152	7	2	27	-3	95	103	4	2	11	0	52	53	3	2	24	2	87	90	4
2	17	-6	92	84	4	2	28	-3	43	44	6	2	12	0	202	194	7	2	25	2	59	67	5
2	19	-6	88	84	4	2	29	-3	68	71	5	2	13	0	234	235	7	2	26	2	96	94	4
2	1	-5	87	94	3	2	0	-2	671	657	5	2	16	0	118	121	5	2	27	2	124	114	5
2	2	-5	162	164	6	2	1	-2	171	164	6	2	18	0	64	67	3	2	28	2	118	115	4
2	3	-5	51	46	4	2	2	-2	143	136	6	2	19	0	66	69	3	2	29	2	96	91	4
2	5	-5	148	142	5	2	3	-2	350	348	6	2	21	0	110	124	4	2	32	2	61	63	5
2	6	-5	93	94	4	2	8	-2	139	143	6	2	22	0	67	80	5	2	2	3	159	162	6
2	8	-5	124	123	5	2	9	-2	43	46	3	2	24	0	78	78	4	2	3	3	44	46	4
2	9	-5	56	59	4	2	10	-2	233	232	7	2	26	0	139	152	6	2	4	3	35	36	4
2	11	-5	88	90	4	2	11	-2	46	44	3	2	28	0	104	115	5	2	5	3	91	89	3
2	12	-5	96	90	4	2	12	-2	132	125	5	2	29	0	102	110	4	2	6	3	139	135	6
2	13	-5	69	67	4	2	16	-2	88	91	4	2	35	0	46	32	6	2	11	3	41	44	4
2	14	-5	101	104	3	2	17	-2	111	116	5	2	1	1	45	41	3	2	12	3	77	78	3
2	16	-5	57	55	5	2	18	-2	61	59	4	2	3	1	72	78	3	2	13	3	50	48	4
2	17	-5	82	79	4	2	20	-2	84	84	4	2	6	1	55	62	3	2	15	3	37	35	6
2	0	-4	537	560	7	2	22	-2	96	101	5	2	7	1	899	858	6	2	16	3	41	42	5
2	1	-4	194	181	7	2	25	-2	82	84	3	2	8	1	61	51	3	2	17	3	140	129	5
2	2	-4	280	298	7	2	26	-2	43	51	6	2	9	1	513	478	6	2	19	3	159	152	7
2	4	-4	149	159	6	2	30	-2	70	71	5	2	10	1	138	127	5	2	22	3	128	127	5
2	5	-4	199	193	7	2	1	-1	254	241	5	2	11	1	153	146	6	2	24	3	46	42	6
2	6	-4	138	135	5	2	2	-1	98	98	4	2	15	1	54	56	3	2	28	3	58	57	6
2	7	-4	280	269	7	2	3	-1	122	121	4	2	16	1	52	55	3	2	32	3	69	60	5
2	9	-4	292	297	8	2	5	-1	476	452	5	2	18	1	107	111	3	2	0	4	99	105	4
2	10	-4	172	167	7	2	6	-1	417	405	5	2	20	1	55	56	5	2	1	4	120	120	5
2	12	-4	118	115	5	2	7	-1	56	57	3	2	21	1	246	247	8	2	2	4	113	110	4
2	14	-4	303	299	8	2	8	-1	120	117	6	2	23	1	606	595	9	2	3	4	236	229	8
2	15	-4	82	93	4	2	10	-1	56	58	3	2	25	1	130	140	6	2	5	4	115	109	5
2	17	-4	92	90	4	2	11	-1	236	224	6	2	28	1	71	80	5	2	7	4	45	45	5
2	20	-4	89	92	4	2	12	-1	158	161	6	2	31	1	88	83	4	2	8	4	66	65	4
2	22	-4	54	53	5	2	14	-1	78	81	3	2	0	2	68	66	3	2	14	4	50	42	5
2	30	-4	58	66	6	2	17	-1	82	83	4	2	1	2	107	103	4	2	16	4	69	72	4
2	32	-4	65	71	6	2	19	-1	69	70	3	2	2	2	77	78	4	2	17	4	137	141	5
2	2	-3	352	340	6	2	21	-1	174	175	7	2	3	2	243	225	7	2	18	4	87	93	4
2	3	-3	297	296	6	2	22	-1	74	96	5	2	4	2	361	355	7	2	21	4	60	63	5

Values of 10*Fobs and 10*Fcalc

$2^2,4^5$-Diphenyl-p-quinquephenyl

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	23	4	96	91	4	3	4	-4	89	88	4	3	24	-2	83	80	4	3	3	1	101	95	4
2	4	5	115	112	4	3	5	-4	72	79	3	3	27	-2	62	64	5	3	4	1	82	85	3
2	5	5	91	93	3	3	7	-4	133	138	6	3	28	-2	63	61	5	3	5	1	95	92	4
2	14	5	40	31	6	3	9	-4	164	160	6	3	29	-2	57	54	7	3	6	1	102	100	4
2	16	5	50	49	5	3	13	-4	88	86	3	3	32	-2	52	42	6	3	7	1	110	108	4
2	19	5	69	76	5	3	14	-4	166	159	5	3	1	-1	36	37	3	3	8	1	47	41	3
2	0	6	114	117	4	3	15	-4	80	85	4	3	2	-1	214	212	7	3	9	1	34	38	4
2	2	6	105	107	4	3	17	-4	138	136	5	3	3	-1	177	157	6	3	14	1	58	59	4
2	4	6	91	90	5	3	18	-4	103	101	4	3	4	-1	183	171	6	3	15	1	43	43	5
2	6	6	97	101	4	3	19	-4	66	64	4	3	5	-1	247	228	7	3	22	1	80	71	4
2	7	6	84	82	4	3	20	-4	54	54	5	3	7	-1	510	471	7	3	23	1	95	95	4
2	9	6	40	30	6	3	21	-4	78	80	4	3	8	-1	68	62	3	3	24	1	78	80	4
2	13	6	45	36	6	3	22	-4	100	106	4	3	9	-1	330	322	7	3	25	1	70	68	4
2	2	7	54	56	6	3	27	-4	48	47	6	3	10	-1	85	83	3	3	27	1	67	59	6
2	4	7	62	72	5	3	1	-3	266	259	7	3	12	-1	53	45	4	3	1	2	103	97	4
2	6	7	48	47	6	3	2	-3	66	65	3	3	13	-1	75	78	3	3	2	2	67	69	3
2	10	7	49	56	6	3	3	-3	305	291	7	3	14	-1	64	79	5	3	3	2	126	125	5
3	0	-8	108	109	5	3	4	-3	94	100	6	3	16	-1	128	125	5	3	4	2	54	53	3
3	9	-8	47	44	6	3	5	-3	150	152	6	3	17	-1	68	65	4	3	7	2	122	117	6
3	11	-8	70	74	5	3	6	-3	274	261	7	3	18	-1	64	67	4	3	8	2	113	106	4
3	6	-7	42	46	6	3	7	-3	115	115	5	3	21	-1	400	382	9	3	9	2	249	240	7
3	13	-7	53	55	5	3	8	-3	84	86	4	3	23	-1	347	338	9	3	10	2	64	63	4
3	16	-7	55	53	5	3	9	-3	33	34	5	3	25	-1	136	138	6	3	14	2	58	51	4
3	0	-6	74	74	4	3	13	-3	41	56	5	3	26	-1	116	144	5	3	16	2	66	62	4
3	1	-6	51	48	5	3	15	-3	83	87	5	3	0	0	100	98	3	3	19	2	85	84	4
3	2	-6	98	103	3	3	19	-3	109	106	5	3	1	0	130	130	5	3	21	2	125	120	4
3	5	-6	75	76	6	3	20	-3	204	225	9	3	3	0	78	79	3	3	22	2	73	74	4
3	7	-6	133	143	7	3	23	-3	146	137	6	3	4	0	345	314	7	3	25	2	99	95	4
3	9	-6	110	104	3	3	24	-3	80	86	5	3	5	0	221	209	7	3	27	2	47	40	6
3	11	-6	45	42	5	3	27	-3	62	56	5	3	6	0	151	148	7	3	28	2	50	43	6
3	12	-6	57	58	5	3	1	-2	112	105	5	3	7	0	161	144	6	3	1	3	37	42	5
3	13	-6	58	57	4	3	2	-2	185	171	6	3	8	0	308	286	7	3	2	3	98	96	4
3	14	-6	68	66	4	3	3	-2	160	149	6	3	9	0	210	189	7	3	5	3	134	143	5
3	18	-6	60	55	4	3	4	-2	118	112	5	3	10	0	358	333	7	3	6	3	60	60	5
3	3	-5	132	140	6	3	6	-2	36	34	4	3	11	0	99	95	3	3	7	3	92	93	4
3	4	-5	146	140	6	3	7	-2	117	118	4	3	12	0	209	193	7	3	13	3	53	51	5
3	5	-5	127	129	5	3	8	-2	194	176	7	3	15	0	113	102	5	3	18	3	62	63	4
3	6	-5	99	96	4	3	9	-2	85	81	4	3	16	0	123	113	5	3	19	3	81	82	3
3	7	-5	70	71	4	3	10	-2	86	86	6	3	17	0	81	80	3	3	23	3	86	83	4
3	9	-5	63	62	4	3	11	-2	122	118	6	3	18	0	100	105	4	3	25	3	55	59	5
3	11	-5	98	102	4	3	12	-2	72	66	3	3	20	0	286	295	9	3	0	4	353	362	9
3	12	-5	78	80	4	3	14	-2	187	185	7	3	21	0	258	252	9	3	2	4	162	165	6
3	14	-5	60	57	4	3	15	-2	128	130	5	3	25	0	134	149	6	3	3	4	128	133	7
3	20	-5	82	80	4	3	16	-2	156	157	5	3	26	0	243	229	8	3	7	4	150	152	7
3	0	-4	271	278	8	3	18	-2	185	182	8	3	28	0	104	104	5	3	9	4	40	39	5
3	1	-4	177	161	7	3	19	-2	116	130	4	3	32	0	57	53	6	3	11	4	43	52	6
3	2	-4	175	166	6	3	20	-2	170	177	7	3	1	1	50	52	3	3	12	4	72	69	4
3	3	-4	150	152	6	3	22	-2	114	110	4	3	2	1	60	61	2	3	16	4	151	149	5

$2^{2},4^{5}$-Diphenyl-p-quinquephenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
3	17	4	52	52	5	4	23	-4	52	61	6	4	10	-1	49	47	4	4	4	3	272	263	10
3	21	4	62	58	5	4	1	-3	42	46	4	4	18	-1	128	131	5	4	5	3	95	97	5
3	1	5	51	49	5	4	2	-3	68	70	3	4	20	-1	123	123	6	4	6	3	40	36	5
3	2	5	146	145	6	4	3	-3	90	89	3	4	21	-1	127	124	4	4	8	3	67	68	4
3	4	5	126	133	6	4	5	-3	64	62	3	4	22	-1	73	73	5	4	9	3	65	68	5
3	6	5	82	85	5	4	7	-3	105	108	3	4	1	0	88	90	3	4	10	3	79	86	4
3	8	5	45	44	6	4	8	-3	54	54	4	4	2	0	112	114	4	4	12	3	92	100	3
3	9	5	65	63	4	4	9	-3	209	199	8	4	3	0	83	83	3	4	14	3	47	55	6
3	10	5	43	49	6	4	11	-3	58	56	4	4	4	0	148	161	6	4	18	3	60	62	5
3	12	5	112	116	5	4	12	-3	86	94	5	4	6	0	105	94	5	4	19	3	50	58	6
3	17	5	103	104	4	4	13	-3	84	86	3	4	7	0	111	111	5	4	5	4	56	62	4
3	10	6	50	51	6	4	14	-3	122	119	4	4	8	0	117	107	5	4	9	4	120	127	4
4	2	-7	44	43	6	4	16	-3	100	99	5	4	10	0	39	39	5	4	10	4	61	60	5
4	0	-6	81	84	4	4	17	-3	171	167	7	4	11	0	66	62	3	4	14	4	54	62	6
4	2	-6	96	96	3	4	18	-3	71	73	4	4	12	0	64	68	3	4	16	4	57	61	5
4	3	-6	81	87	4	4	19	-3	104	98	4	4	15	0	38	37	5	4	5	5	97	100	5
4	4	-6	64	69	4	4	20	-3	50	56	6	4	18	0	51	55	5	4	7	5	43	32	6
4	5	-6	50	53	5	4	21	-3	199	197	8	4	19	0	106	107	4	4	9	5	55	55	5
4	7	-6	168	169	6	4	23	-3	140	141	6	4	22	0	167	165	7	5	3	-8	53	51	6
4	8	-6	55	54	5	4	25	-3	94	92	4	4	23	0	85	97	5	5	5	-7	73	72	5
4	9	-6	122	128	4	4	0	-2	66	64	3	4	27	0	55	60	6	5	6	-7	74	82	6
4	12	-6	44	44	6	4	1	-2	39	49	4	4	2	1	96	96	4	5	7	-7	71	79	5
4	14	-6	58	57	5	4	2	-2	79	75	4	4	3	1	60	62	3	5	8	-7	108	120	4
4	15	-6	61	52	5	4	3	-2	47	51	4	4	4	1	117	117	6	5	10	-7	52	46	6
4	19	-6	53	54	6	4	4	-2	230	220	8	4	5	1	80	78	3	5	11	-7	67	61	5
4	5	-5	147	152	7	4	5	-2	99	97	4	4	11	1	39	44	5	5	6	-6	49	50	6
4	6	-5	158	158	7	4	6	-2	71	70	3	4	19	1	84	91	5	5	10	-6	58	71	5
4	7	-5	144	146	6	4	7	-2	68	70	3	4	26	1	55	52	5	5	15	-6	69	69	5
4	8	-5	173	169	6	4	8	-2	53	53	4	4	29	1	64	55	5	5	9	-5	109	113	4
4	11	-5	60	59	4	4	9	-2	35	28	5	4	0	2	517	508	8	5	10	-5	52	45	5
4	12	-5	109	115	4	4	10	-2	126	122	5	4	1	2	96	86	4	5	12	-5	85	82	4
4	14	-5	41	44	6	4	11	-2	58	56	4	4	2	2	234	223	8	5	14	-5	95	92	4
4	18	-5	86	83	4	4	12	-2	134	126	5	4	3	2	141	136	4	5	21	-5	63	63	5
4	20	-5	91	95	4	4	14	-2	103	94	5	4	4	2	107	109	3	5	3	-4	61	63	4
4	21	-5	99	96	5	4	15	-2	46	47	5	4	8	2	111	105	4	5	6	-4	77	84	5
4	23	-5	89	89	4	4	18	-2	272	273	9	4	10	2	84	85	3	5	12	-4	114	117	4
4	0	-4	117	116	4	4	19	-2	105	101	4	4	13	2	46	49	5	5	14	-4	45	51	6
4	1	-4	68	66	3	4	20	-2	127	131	5	4	14	2	90	96	3	5	16	-4	64	57	4
4	3	-4	83	76	3	4	21	-2	51	56	5	4	16	2	161	171	7	5	18	-4	95	91	4
4	4	-4	97	92	4	4	22	-2	86	86	4	4	17	2	67	66	4	5	20	-4	86	85	4
4	5	-4	62	65	4	4	24	-2	116	115	4	4	18	2	49	52	5	5	1	-3	110	109	4
4	6	-4	89	88	4	4	25	-2	82	90	5	4	20	2	80	82	4	5	2	-3	66	67	4
4	8	-4	57	53	4	4	26	-2	69	76	5	4	21	2	70	69	4	5	3	-3	85	84	4
4	9	-4	50	53	5	4	28	-2	90	96	4	4	23	2	63	66	5	5	5	-3	42	37	5
4	12	-4	115	125	6	4	1	-1	75	67	4	4	25	2	44	39	6	5	6	-3	101	109	5
4	15	-4	71	68	4	4	5	-1	83	80	3	4	26	2	55	60	6	5	8	-3	40	39	6
4	16	-4	119	122	4	4	6	-1	155	141	5	4	2	3	129	134	5	5	9	-3	121	123	6
4	17	-4	103	114	5	4	7	-1	70	69	3	4	3	3	208	213	7	5	14	-3	65	71	4

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
5	15	-3	94	92	4	5	9	2	60	63	4	7	5	-3	80	82	5						
5	16	-3	98	95	3	5	2	3	133	129	4	7	9	-3	60	63	5						
5	19	-3	73	72	5	5	14	3	69	66	4	7	9	-2	60	59	5						
5	22	-3	66	65	5	6	14	-5	48	52	6	7	4	-1	54	62	6						
5	0	-2	171	174	7	6	16	-5	88	87	5	7	5	-1	65	74	5						
5	1	-2	115	112	4	6	17	-5	52	39	6												
5	3	-2	132	131	6	6	0	-4	138	145	5												
5	4	-2	144	135	6	6	2	-4	64	68	4												
5	6	-2	42	38	5	6	3	-4	93	98	4												
5	8	-2	107	102	4	6	5	-4	54	60	5												
5	10	-2	52	46	4	6	12	-4	95	99	4												
5	12	-2	55	55	4	6	15	-4	97	98	4												
5	15	-2	72	76	5	6	16	-4	85	86	5												
5	16	-2	77	78	4	6	17	-4	60	64	6												
5	17	-2	105	106	4	6	1	-3	60	61	4												
5	18	-2	64	72	5	6	7	-3	72	70	4												
5	24	-2	49	41	6	6	11	-3	64	58	4												
5	1	-1	142	144	5	6	12	-3	49	45	6												
5	2	-1	70	69	3	6	0	-2	75	67	4												
5	3	-1	140	136	6	6	2	-2	193	186	7												
5	5	-1	139	144	6	6	4	-2	51	46	5												
5	6	-1	50	50	5	6	5	-2	67	68	4												
5	7	-1	101	101	6	6	6	-2	112	116	5												
5	8	-1	82	85	4	6	9	-2	73	71	4												
5	9	-1	109	118	5	6	10	-2	105	111	4												
5	10	-1	52	45	4	6	11	-2	54	60	5												
5	11	-1	47	57	5	6	12	-2	75	79	4												
5	13	-1	42	37	5	6	14	-2	99	94	4												
5	0	0	335	347	10	6	3	-1	145	144	6												
5	2	0	210	226	8	6	4	-1	104	101	4												
5	3	0	146	154	6	6	5	-1	166	168	8												
5	4	0	52	51	4	6	9	-1	77	82	4												
5	9	0	97	97	3	6	11	-1	81	114	11												
5	10	0	57	60	4	6	18	-1	48	55	6												
5	14	0	117	116	4	6	0	0	74	87	4												
5	16	0	110	121	5	6	1	0	110	121	5												
5	1	1	78	74	4	6	2	0	71	85	4												
5	2	1	262	255	10	6	5	0	68	73	4												
5	3	1	323	316	9	6	11	0	54	57	5												
5	4	1	80	74	4	6	13	0	53	52	5												
5	5	1	146	148	6	6	1	1	80	75	4												
5	8	1	38	41	6	6	3	1	52	58	5												
5	13	1	92	91	3	6	4	1	72	77	4												
5	14	1	87	86	4	6	1	2	101	100	5												
5	15	1	44	40	5	6	3	3	65	62	6												
5	18	1	97	101	4	6	5	3	45	46	6												
5	19	1	67	72	5	7	5	-4	50	43	6												
5	7	2	56	58	4	7	3	-3	67	65	5												

Appendix B

$2^2,6^5$-Diphenyl-p-septiphenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
0	1	-7	66	62	3	0	8	-5	23	23	5	5	-2	-5	117	117	4	3	-3	-4	33	31	4
0	2	-7	39	40	4	0	10	-5	41	38	3	5	-1	-5	249	248	5	3	1	-4	48	48	2
2	0	-7	35	35	4	0	12	-5	61	58	4	5	0	-5	45	46	3	3	2	-4	111	114	3
3	2	-7	61	58	4	1	-6	-5	29	33	4	5	3	-5	122	125	5	3	3	-4	223	221	4
4	0	-7	71	70	3	1	0	-5	37	43	4	5	4	-5	91	92	4	3	7	-4	25	17	5
0	2	-6	26	33	5	1	3	-5	48	45	3	5	6	-5	31	26	4	3	8	-4	95	100	3
0	4	-6	33	34	4	1	4	-5	75	77	2	5	8	-5	39	40	3	4	-7	-4	28	32	4
0	5	-6	37	37	3	1	5	-5	170	165	5	5	9	-5	51	46	3	4	-6	-4	55	56	2
0	9	-6	161	151	5	1	6	-5	62	63	3	6	1	-5	70	72	3	4	-5	-4	27	30	4
0	10	-6	107	98	5	1	8	-5	62	60	2	6	5	-5	61	68	4	4	-4	-4	43	41	3
1	-4	-6	39	41	4	1	9	-5	80	84	6	6	6	-5	78	80	4	4	0	-4	78	86	3
1	-3	-6	37	38	4	1	10	-5	119	121	5	7	-7	-5	51	48	3	4	5	-4	32	33	4
1	0	-6	32	34	4	1	12	-5	28	27	4	7	3	-5	26	27	4	4	7	-4	31	25	4
1	1	-6	85	89	3	2	-4	-5	25	24	5	8	-5	-5	36	36	4	4	8	-4	74	76	2
1	6	-6	88	93	4	2	-3	-5	51	64	3	8	-3	-5	25	18	5	4	9	-4	194	198	5
1	7	-6	68	63	2	2	-2	-5	41	41	3	8	-2	-5	46	41	3	4	10	-4	40	42	3
1	10	-6	27	22	5	2	-1	-5	43	43	3	8	-1	-5	62	63	3	5	-8	-4	98	106	5
2	-1	-6	78	76	3	2	0	-5	68	65	3	8	0	-5	30	37	4	5	-7	-4	50	53	3
2	0	-6	85	79	4	2	1	-5	69	68	2	8	7	-5	25	20	5	5	-3	-4	25	28	5
2	1	-6	73	75	3	2	2	-5	139	141	5	9	6	-5	28	27	5	5	-2	-4	49	58	5
2	3	-6	44	42	3	2	5	-5	57	57	2	11	1	-5	27	26	5	5	0	-4	84	89	3
2	4	-6	76	78	3	2	6	-5	38	38	3	0	1	-4	101	98	4	5	1	-4	119	127	5
2	8	-6	60	61	3	2	7	-5	105	104	3	0	2	-4	27	31	4	5	2	-4	75	73	3
2	9	-6	38	39	4	2	8	-5	75	71	3	0	4	-4	68	73	4	5	3	-4	49	48	3
3	-2	-6	27	14	5	2	9	-5	38	33	3	0	5	-4	67	63	3	5	4	-4	29	28	4
3	1	-6	99	100	4	2	11	-5	59	61	3	0	6	-4	54	57	2	5	6	-4	44	43	3
3	4	-6	33	31	4	2	12	-5	70	75	4	0	7	-4	27	35	4	5	7	-4	76	75	3
3	5	-6	72	63	4	2	13	-5	26	25	5	0	9	-4	67	63	3	5	8	-4	62	62	3
3	6	-6	139	147	6	3	-6	-5	98	103	3	0	10	-4	59	59	2	6	-11	-4	52	52	3
4	-6	-6	29	22	5	3	-5	-5	46	45	3	0	11	-4	127	124	5	6	-10	-4	32	37	4
4	-1	-6	72	71	2	3	-2	-5	36	36	3	0	12	-4	62	60	3	6	-6	-4	34	38	3
4	0	-6	50	57	4	3	0	-5	106	105	5	1	-7	-4	54	53	2	6	-4	-4	59	58	2
4	1	-6	43	37	3	3	2	-5	41	40	3	1	3	-4	120	117	4	6	-3	-4	100	106	5
4	2	-6	25	25	5	3	4	-5	151	159	5	1	4	-4	102	90	3	6	-2	-4	106	112	5
4	3	-6	60	59	3	3	5	-5	50	48	3	1	8	-4	120	111	5	6	-1	-4	346	350	5
5	-5	-6	31	27	5	3	9	-5	93	98	4	1	9	-4	193	195	5	6	0	-4	126	128	5
5	0	-6	90	91	2	3	10	-5	45	45	3	1	10	-4	90	88	3	6	1	-4	53	51	3
6	-3	-6	42	31	4	4	-9	-5	38	46	4	1	11	-4	34	39	3	6	6	-4	28	26	4
6	-2	-6	48	46	3	4	-8	-5	37	45	4	2	-2	-4	26	19	4	6	7	-4	30	27	4
7	-1	-6	48	45	3	4	-6	-5	31	25	4	2	1	-4	28	25	3	6	8	-4	43	41	3
8	-3	-6	43	43	4	4	-4	-5	39	42	3	2	2	-4	38	39	3	6	9	-4	52	60	3
8	-1	-6	27	19	5	4	-3	-5	62	61	3	2	3	-4	90	88	4	6	10	-4	31	30	4
0	1	-5	70	65	4	4	-2	-5	33	35	4	2	4	-4	52	45	2	7	-6	-4	35	37	3
0	2	-5	42	50	3	4	-1	-5	80	83	3	2	5	-4	55	52	3	7	-5	-4	31	29	4
0	3	-5	109	115	5	4	1	-5	217	218	5	2	10	-4	133	133	5	7	-4	-4	214	218	5
0	5	-5	24	29	5	4	2	-5	151	152	5	2	11	-4	46	44	3	7	-3	-4	194	186	5
0	6	-5	43	35	3	4	6	-5	98	88	4	3	-8	-4	25	23	4	7	-2	-4	55	52	3
0	7	-5	58	56	2	4	11	-5	40	34	3	3	-4	-4	28	26	4	7	6	-4	136	142	5

$2^2,6^5$-Diphenyl-p-septiphenyl

Values of 10*Fobs and 10*Fcalc

H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF
7 7 -4	30	24	4	2 -2 -3	63	65	3	4 13 -3	122	118	4	9 -6 -3	140	132	5
7 8 -4	36	35	3	2 -1 -3	111	107	3	5-10 -3	69	67	3	9 -5 -3	86	84	3
7 9 -4	34	32	4	2 0 -3	36	32	2	5 -9 -3	46	54	3	9 -4 -3	51	52	2
8 -7 -4	42	39	3	2 1 -3	25	27	3	5 -5 -3	28	31	3	9 -3 -3	33	33	3
8 -5 -4	26	20	4	2 2 -3	86	85	3	5 -1 -3	26	17	3	9 -2 -3	71	76	3
8 -1 -4	38	38	3	2 3 -3	214	205	4	5 1 -3	66	68	2	9 -1 -3	113	111	5
8 0 -4	37	33	3	2 4 -3	262	250	4	5 5 -3	49	49	2	9 3 -3	71	77	2
8 2 -4	42	41	3	2 5 -3	108	104	4	5 7 -3	38	38	3	9 4 -3	82	89	3
8 3 -4	95	108	4	2 8 -3	43	43	2	5 8 -3	89	83	3	10 -9 -3	59	61	3
8 4 -4	75	89	4	2 9 -3	295	296	5	5 9 -3	108	107	4	10 -8 -3	23	26	5
9 -6 -4	44	39	3	2 10 -3	60	63	2	5 10 -3	39	40	3	10 -7 -3	45	43	3
9 -5 -4	85	89	4	2 11 -3	25	28	4	5 11 -3	35	37	3	10 -4 -3	70	77	4
9 1 -4	50	58	3	2 13 -3	38	42	3	6-12 -3	38	35	4	10 -3 -3	41	45	3
9 6 -4	39	40	3	2 14 -3	77	79	3	6 -8 -3	52	52	2	10 0 -3	38	42	3
9 7 -4	37	41	4	3-11 -3	33	38	4	6 -7 -3	30	33	4	10 1 -3	87	99	5
9 8 -4	48	44	3	3-10 -3	48	50	3	6 -1 -3	39	38	2	10 2 -3	58	56	2
10 -8 -4	52	49	3	3 -9 -3	117	111	5	6 0 -3	59	57	4	10 3 -3	30	33	4
10 -7 -4	73	67	3	3 -7 -3	30	27	4	6 1 -3	67	61	3	11 -7 -3	74	68	3
10 4 -4	25	16	5	3 -5 -3	23	17	4	6 2 -3	170	163	5	11 -3 -3	26	29	4
11 -2 -4	26	21	5	3 -2 -3	45	48	2	6 3 -3	59	60	2	11 -2 -3	43	39	3
0 3 -3	53	49	2	3 -1 -3	58	58	2	6 -7 -3	69	72	3	11 0 -3	26	30	4
0 4 -3	124	110	4	3 0 -3	78	79	2	6 8 -3	33	28	3	0 2 -2	93	86	4
0 5 -3	111	110	4	3 1 -3	78	79	4	7-10 -3	91	86	3	0 3 -2	61	61	3
0 6 -3	69	63	2	3 2 -3	233	221	4	7 -6 -3	32	33	4	0 4 -2	64	68	2
0 8 -3	91	93	3	3 3 -3	162	165	4	7 -5 -3	116	112	4	0 5 -2	39	40	3
0 9 -3	161	164	5	3 4 -3	100	101	4	7 -4 -3	89	91	3	0 7 -2	30	38	3
0 14 -3	76	73	4	3 5 -3	54	51	3	7 -3 -3	60	58	3	0 8 -2	59	59	2
0 15 -3	83	76	3	3 6 -3	243	232	4	7 -1 -3	108	111	3	0 9 -2	51	51	2
1 -4 -3	44	47	2	3 7 -3	65	63	2	7 0 -3	55	52	2	0 10 -2	66	67	3
1 -3 -3	392	378	4	3 9 -3	46	45	3	7 6 -3	51	55	3	0 11 -2	61	57	2
1 -2 -3	41	38	2	3 10 -3	119	116	4	7 7 -3	45	44	3	0 12 -2	37	46	3
1 1 -3	36	32	2	3 11 -3	179	172	5	7 8 -3	38	37	3	0 13 -2	67	74	4
1 2 -3	76	78	2	3 12 -3	32	40	4	7 9 -3	44	42	3	1-12 -2	49	43	2
1 3 -3	158	153	4	3 13 -3	25	11	4	7 10 -3	27	31	5	1-11 -2	52	53	2
1 4 -3	125	116	4	3 14 -3	33	32	4	8-10 -3	65	59	2	1-10 -2	158	166	6
1 6 -3	119	114	5	4 -7 -3	35	30	3	8 -9 -3	72	67	3	1 -9 -2	360	363	5
1 7 -3	163	157	4	4 -6 -3	35	36	3	8 -8 -3	120	124	6	1 -8 -2	49	51	3
1 8 -3	25	22	4	4 -5 -3	67	65	3	8 -4 -3	151	160	6	1 -6 -2	19	18	4
1 9 -3	92	86	3	4 -4 -3	97	93	3	8 -3 -3	251	249	5	1 -5 -2	36	37	2
1 10 -3	50	53	2	4 -3 -3	89	90	3	8 -2 -3	58	61	2	1 -3 -2	39	40	2
2-11 -3	47	45	3	4 -2 -3	88	85	4	8 -1 -3	44	45	3	1 -2 -2	24	25	3
2-10 -3	38	31	3	4 0 -3	46	40	2	8 2 -3	47	42	3	1 -1 -2	73	74	3
2 -9 -3	49	46	2	4 1 -3	38	38	2	8 3 -3	37	37	3	1 0 -2	212	210	3
2 -8 -3	29	22	4	4 3 -3	35	29	2	8 6 -3	23	26	4	1 1 -2	23	20	3
2 -6 -3	47	45	3	4 7 -3	25	25	4	8 7 -3	36	41	3	1 2 -2	59	60	3
2 -5 -3	32	25	3	4 8 -3	286	276	5	9 -9 -3	34	38	4	1 3 -2	120	124	4
2 -4 -3	31	29	3	4 9 -3	55	53	3	9 -8 -3	31	27	4	1 4 -2	138	136	4
2 -3 -3	69	74	4	4 12 -3	41	39	3	9 -7 -3	62	61	2	1 5 -2	141	133	4

$2^2,6^5$-Diphenyl-p-septiphenyl

Values of 10*Fobs and 10*Fcalc

H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF
1 7 -2	35	38	2	4-11 -2	30	32	4	7 -2 -2	279	281	4	12 -4 -2	75	78	3
1 8 -2	43	48	2	4-10 -2	49	49	2	7 2 -2	78	75	4	12 -3 -2	34	32	3
1 9 -2	25	25	5	4 -8 -2	88	84	3	7 4 -2	33	34	3	12 -2 -2	36	42	3
1 14 -2	35	38	3	4 -6 -2	37	37	2	7 5 -2	59	59	3	0 1 -1	218	219	2
1 15 -2	66	66	4	4 -4 -2	72	66	2	7 7 -2	26	28	4	0 2 -1	263	270	2
2-13 -2	86	82	2	4 -2 -2	36	42	2	7 8 -2	31	33	3	0 3 -1	146	148	3
2-12 -2	161	158	5	4 -1 -2	20	17	3	7 10 -2	29	23	4	0 5 -1	41	46	1
2-11 -2	40	34	3	4 0 -2	97	94	4	8-10 -2	33	43	3	0 6 -1	290	274	3
2-10 -2	59	62	3	4 1 -2	403	384	3	8 -9 -2	37	44	3	0 7 -1	183	185	4
2 -8 -2	51	58	2	4 2 -2	560	531	3	8 -5 -2	64	65	3	0 8 -1	41	41	2
2 -7 -2	97	102	5	4 3 -2	41	42	2	8 -4 -2	77	79	3	0 9 -1	50	52	2
2 -6 -2	35	31	2	4 6 -2	99	96	4	8 -3 -2	21	23	4	0 10 -1	52	51	2
2 -4 -2	124	126	4	4 7 -2	73	72	2	8 -2 -2	32	26	3	0 11 -1	76	72	2
2 -3 -2	545	542	3	4 9 -2	53	53	3	8 0 -2	63	59	3	1-10 -1	137	136	5
2 -2 -2	258	262	3	4 11 -2	117	124	5	8 2 -2	50	48	2	1 -9 -1	77	86	4
2 -1 -2	18	10	3	4 12 -2	94	95	4	8 3 -2	61	67	3	1 -8 -1	25	25	3
2 0 -2	38	37	3	5 -9 -2	41	37	3	8 4 -2	43	47	3	1 -6 -1	224	223	4
2 1 -2	91	95	3	5 -8 -2	27	32	4	8 5 -2	64	63	3	1 -1 -1	18	18	3
2 2 -2	65	60	2	5 -6 -2	61	67	2	8 8 -2	30	23	4	1 0 -1	59	61	2
2 4 -2	56	56	1	5 -5 -2	90	86	5	8 9 -2	42	37	3	1 1 -1	96	97	3
2 5 -2	74	70	3	5 -4 -2	54	53	3	9-11 -2	38	33	3	1 2 -1	250	252	2
2 7 -2	87	82	2	5 -3 -2	39	39	2	9 -8 -2	96	91	4	1 3 -1	186	196	3
2 8 -2	29	33	3	5 -2 -2	101	102	3	9 -3 -2	148	149	5	1 4 -1	22	23	3
2 9 -2	41	42	3	5 -1 -2	215	202	4	9 -2 -2	21	8	5	1 5 -1	188	175	3
2 10 -2	23	28	4	5 0 -2	42	41	2	9 -1 -2	35	36	3	1 6 -1	215	210	3
2 12 -2	152	153	6	5 1 -2	92	90	3	9 2 -2	62	60	3	1 7 -1	167	163	4
2 13 -2	45	45	3	5 2 -2	60	57	3	9 3 -2	85	87	3	1 8 -1	46	47	3
3-12 -2	24	26	4	5 5 -2	58	63	2	9 4 -2	61	71	5	1 13 -1	71	76	3
3-11 -2	47	49	3	5 6 -2	53	54	3	9 6 -2	31	26	3	1 14 -1	54	56	3
3-10 -2	152	161	5	5 8 -2	296	307	5	9 7 -2	71	73	4	2-15 -1	59	53	3
3 -9 -2	65	64	3	5 9 -2	287	293	5	9 8 -2	24	10	5	2-14 -1	82	73	3
3 -8 -2	28	31	4	5 13 -2	72	56	4	10-11 -2	71	69	3	2-10 -1	71	70	3
3 -6 -2	199	200	4	6-13 -2	40	39	3	10-10 -2	90	95	4	2 -9 -1	142	158	5
3 -5 -2	303	289	4	6-12 -2	46	47	3	10 -9 -2	27	26	4	2 -8 -1	65	64	3
3 -4 -2	81	76	4	6-11 -2	56	59	3	10 -6 -2	75	77	4	2 -7 -1	27	22	3
3 -3 -2	101	98	4	6-10 -2	50	47	3	10 -5 -2	69	73	3	2 -6 -1	42	44	2
3 -2 -2	34	35	2	6 -9 -2	26	20	4	10 -4 -2	67	71	3	2 -4 -1	136	131	3
3 -1 -2	30	33	2	6 -3 -2	39	39	2	10 -3 -2	108	104	4	2 -3 -1	118	117	4
3 1 -2	78	75	4	6 1 -2	59	59	2	10 -2 -2	54	54	2	2 -2 -1	238	239	3
3 2 -2	142	140	3	6 4 -2	40	36	2	10 -1 -2	41	38	3	2 -1 -1	443	452	2
3 3 -2	53	50	2	6 5 -2	86	81	4	10 3 -2	39	41	3	2 0 -1	660	676	2
3 4 -2	277	269	3	6 6 -2	343	343	4	11 -8 -2	45	42	3	2 1 -1	35	34	2
3 5 -2	204	205	4	6 7 -2	60	64	2	11 -4 -2	123	128	5	2 2 -1	129	129	3
3 7 -2	40	39	2	6 8 -2	73	75	2	11 -3 -2	91	90	4	2 3 -1	50	50	2
3 10 -2	61	58	3	6 9 -2	37	35	3	11 1 -2	29	27	4	2 4 -1	104	105	3
4-14 -2	35	34	4	6 10 -2	45	45	3	11 2 -2	60	62	2	2 5 -1	34	37	2
4-13 -2	56	51	3	6 11 -2	75	72	3	12 -6 -2	53	49	3	2 6 -1	35	31	2
4-12 -2	37	41	3	7 -5 -2	28	25	3	12 -5 -2	33	37	4	2 7 -1	28	27	3

Appendix B

$2^2,6^5$-Diphenyl-p-septiphenyl

Values of 10*Fobs and 10*Fcalc

H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF
2 11 -1	85	98	3	5-10 -1	41	40	3	8 -7 -1	33	28	3	13 -5 -1	68	66	3
2 12 -1	31	34	3	5 -8 -1	152	147	5	8 -6 -1	96	91	4	0 1 0	177	180	4
3-13 -1	45	41	3	5 -7 -1	87	90	5	8 -5 -1	22	9	4	0 2 0	24	29	2
3-12 -1	163	157	5	5 -5 -1	60	56	2	8 -4 -1	106	109	4	0 3 0	67	65	3
3-11 -1	166	161	5	5 -4 -1	42	41	2	8 -3 -1	122	128	5	0 4 0	188	183	7
3-10 -1	23	19	4	5 -3 -1	138	145	4	8 -2 -1	165	178	5	0 5 0	89	85	4
3 -9 -1	69	68	2	5 -2 -1	316	327	3	8 -1 -1	65	70	2	0 6 0	66	69	3
3 -8 -1	75	76	3	5 -1 -1	338	339	3	8 0 -1	21	27	4	0 8 0	61	63	2
3 -7 -1	101	96	4	5 0 -1	269	267	3	8 1 -1	45	43	2	0 9 0	84	83	3
3 -6 -1	61	62	2	5 1 -1	211	205	3	8 3 -1	173	173	5	0 10 0	77	75	7
3 -5 -1	79	73	2	5 2 -1	312	305	3	8 4 -1	266	268	5	0 11 0	25	25	5
3 -4 -1	63	64	3	5 3 -1	52	46	2	8 5 -1	33	35	3	0 12 0	37	47	3
3 -2 -1	274	273	3	5 6 -1	50	54	2	8 7 -1	35	32	3	1 -8 0	207	207	6
3 -1 -1	190	194	3	5 7 -1	41	34	2	8 8 -1	45	48	3	1 -7 0	142	137	4
3 0 -1	66	66	2	5 13 -1	31	34	4	9 -9 -1	85	88	2	1 -6 0	191	179	6
3 1 -1	27	24	2	6-11 -1	22	27	4	9 -8 -1	25	28	4	1 -5 0	130	119	3
3 3 -1	86	76	3	6 -8 -1	68	70	2	9 -5 -1	118	120	4	1 -3 0	1144	1187	7
3 4 -1	106	109	4	6 -7 -1	75	76	3	9 -4 -1	189	187	5	1 -2 0	515	528	2
3 5 -1	105	95	4	6 -4 -1	115	112	4	9 -2 -1	31	28	3	1 -1 0	152	159	2
3 6 -1	90	85	3	6 -3 -1	109	103	4	9 -1 -1	60	62	2	1 0 0	203	207	2
3 7 -1	71	73	3	6 -2 -1	49	43	2	9 1 -1	133	139	5	1 1 0	231	245	2
3 8 -1	33	27	3	6 -1 -1	378	365	4	9 2 -1	61	61	2	1 2 0	84	86	3
3 9 -1	23	28	4	6 0 -1	211	190	4	10-12 -1	25	29	5	1 4 0	79	72	3
3 11 -1	23	30	4	6 2 -1	24	19	3	10 -7 -1	84	82	3	1 5 0	218	198	4
3 12 -1	93	99	3	6 3 -1	52	53	3	10 -6 -1	23	24	4	1 6 0	320	308	3
4-15 -1	62	61	3	6 4 -1	192	195	4	10 -4 -1	96	93	5	1 7 0	316	314	6
4-12 -1	43	43	3	6 5 -1	57	53	2	10 -3 -1	125	127	5	1 8 0	134	135	4
4-10 -1	211	219	5	6 7 -1	44	43	3	10 -2 -1	51	42	2	1 9 0	48	48	2
4 -9 -1	139	143	4	6 8 -1	106	105	4	10 0 -1	43	41	2	2-11 0	179	185	14
4 -8 -1	87	88	4	6 9 -1	175	175	6	10 2 -1	85	92	4	2-10 0	145	144	4
4 -7 -1	62	62	2	7-14 -1	51	50	4	10 3 -1	131	131	3	2 -9 0	46	47	3
4 -6 -1	110	105	4	7-13 -1	42	43	4	10 6 -1	22	7	5	2 -8 0	92	91	4
4 -5 -1	313	304	3	7 -9 -1	46	46	3	10 8 -1	36	37	4	2 -7 0	58	54	3
4 -4 -1	191	183	3	7 -7 -1	33	29	3	11-10 -1	59	60	2	2 -6 0	67	64	2
4 -3 -1	102	100	4	7 -6 -1	29	25	3	11 -6 -1	50	53	3	2 -5 0	94	98	3
4 -2 -1	139	142	3	7 -5 -1	53	48	2	11 -5 -1	74	69	2	2 -4 0	205	208	3
4 -1 -1	219	222	3	7 -4 -1	230	234	4	11 -4 -1	81	80	4	2 -3 0	133	132	4
4 0 -1	170	173	3	7 -2 -1	133	136	5	11 -3 -1	76	75	3	2 -2 0	79	83	4
4 1 -1	106	110	4	7 -1 -1	168	169	4	11 -1 -1	26	27	4	2 -1 0	137	138	2
4 3 -1	18	15	3	7 0 -1	96	95	4	11 0 -1	134	133	5	2 0 0	350	358	2
4 4 -1	72	72	3	7 1 -1	158	151	4	11 1 -1	44	45	3	2 1 0	381	385	2
4 5 -1	79	90	3	7 2 -1	108	111	4	11 2 -1	58	60	2	2 2 0	178	184	3
4 6 -1	119	109	5	7 5 -1	51	50	3	11 3 -1	25	15	4	2 3 0	95	81	3
4 7 -1	64	67	2	7 6 -1	369	375	5	12 -5 -1	46	49	3	2 4 0	349	346	3
4 9 -1	26	29	4	7 7 -1	206	203	5	12 -4 -1	78	79	4	2 5 0	393	386	3
4 10 -1	81	78	3	7 8 -1	38	36	3	12 -1 -1	31	34	4	2 6 0	175	170	4
5-12 -1	82	84	3	8-10 -1	33	36	3	12 2 -1	24	23	5	2 7 0	35	30	2
5-11 -1	23	23	4	8 -9 -1	24	30	4	13 -6 -1	51	51	3	2 9 0	54	46	3

$2^2,6^5$-Diphenyl-p-septiphenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
2	14	0	79	78	3	5	-1	0	164	159	3	9	0	0	80	75	4	1	-3	1	157	161	3
3	-13	0	57	57	2	5	0	0	138	133	3	9	1	0	53	53	2	1	-2	1	54	50	2
3	-12	0	48	54	3	5	3	0	40	36	2	9	3	0	99	95	4	1	-1	1	252	252	2
3	-11	0	63	61	2	5	4	0	49	48	3	9	4	0	178	173	9	1	0	1	1113	1181	7
3	-9	0	54	53	2	6	-13	0	53	54	3	9	5	0	95	95	4	1	1	1	466	485	2
3	-6	0	59	58	2	6	-12	0	162	167	8	9	6	0	69	70	3	1	3	1	56	54	2
3	-5	0	89	90	4	6	-11	0	70	68	3	9	9	0	45	41	3	1	4	1	48	56	3
3	-4	0	506	507	3	6	-10	0	59	63	2	10	-9	0	92	95	6	1	7	1	28	26	3
3	-3	0	675	692	5	6	-8	0	103	101	4	10	-8	0	48	50	3	1	8	1	46	45	2
3	-2	0	591	604	5	6	-7	0	52	46	3	10	-7	0	33	31	3	1	9	1	76	83	3
3	-1	0	573	585	6	6	-6	0	95	89	5	10	-3	0	48	48	2	1	11	1	60	60	3
3	0	0	378	381	6	6	-5	0	38	35	2	10	-2	0	52	52	6	2	-14	1	26	33	4
3	1	0	62	62	3	6	-4	0	90	89	4	10	1	0	163	166	8	2	-13	1	53	55	2
3	2	0	137	127	3	6	-3	0	124	124	4	10	2	0	50	53	3	2	-12	1	64	65	3
3	3	0	82	84	3	6	-2	0	142	139	4	10	6	0	126	126	12	2	-10	1	25	21	3
3	4	0	32	32	2	6	-1	0	102	99	4	10	7	0	27	27	5	2	-8	1	49	51	2
3	5	0	94	94	4	6	0	0	48	47	3	11	-11	0	62	64	4	2	-7	1	485	489	3
3	6	0	57	56	3	6	2	0	55	57	2	11	-7	0	54	55	3	2	-6	1	43	44	2
3	10	0	33	33	3	6	3	0	34	34	2	11	-6	0	55	53	3	2	-5	1	142	146	3
3	11	0	130	133	6	6	5	0	23	19	4	11	-5	0	37	37	3	2	-4	1	153	158	3
3	12	0	35	33	3	6	7	0	84	83	5	11	-4	0	39	38	5	2	-3	1	854	874	2
4	-12	0	81	92	9	7	-14	0	41	41	3	11	-2	0	145	141	5	2	-2	1	1277	1324	8
4	-11	0	97	103	4	7	-9	0	58	57	2	11	-1	0	64	68	3	2	-1	1	162	162	3
4	-10	0	100	94	4	7	-8	0	56	57	3	11	4	0	64	59	3	2	0	1	218	222	3
4	-9	0	111	110	4	7	-3	0	49	48	2	11	5	0	48	46	5	2	1	1	22	24	3
4	-8	0	113	112	4	7	-2	0	64	70	2	12	-5	0	132	128	4	2	2	1	148	147	3
4	-7	0	236	230	4	7	-1	0	161	154	4	12	-4	0	136	133	10	2	3	1	207	210	3
4	-6	0	229	232	4	7	0	0	136	141	4	12	-3	0	39	42	4	2	4	1	100	103	4
4	-4	0	27	28	2	7	2	0	23	23	3	12	0	0	80	77	4	2	5	1	66	66	3
4	-3	0	64	65	3	7	3	0	54	53	3	12	1	0	55	56	3	2	7	1	202	197	4
4	-2	0	94	94	3	7	6	0	52	51	2	13	-7	0	91	92	11	2	8	1	47	57	2
4	0	0	123	121	3	7	7	0	85	85	3	13	-5	0	69	69	3	2	9	1	67	67	3
4	1	0	33	29	2	7	10	0	49	47	3	13	-3	0	36	34	5	2	10	1	33	39	3
4	2	0	79	80	3	8	-8	0	35	41	3	13	-2	0	78	81	3	3	-16	1	29	31	4
4	3	0	139	131	7	8	-7	0	33	28	3	0	0	1	57	61	3	3	-15	1	44	41	3
4	4	0	35	29	2	8	-5	0	58	57	2	0	2	1	33	31	2	3	-14	1	43	45	3
4	9	0	68	69	5	8	-4	0	109	105	5	0	3	1	264	248	3	3	-13	1	50	53	2
5	-15	0	39	39	7	8	-2	0	97	93	4	0	4	1	165	159	3	3	-11	1	68	66	2
5	-13	0	82	85	3	8	0	0	55	54	5	0	6	1	26	29	3	3	-10	1	48	51	2
5	-12	0	45	47	2	8	1	0	144	143	5	0	8	1	67	68	2	3	-8	1	82	79	4
5	-10	0	85	83	4	8	2	0	159	165	5	0	9	1	65	68	2	3	-7	1	69	73	3
5	-9	0	104	105	5	8	6	0	155	150	6	1	-13	1	38	40	3	3	-6	1	182	189	3
5	-8	0	20	22	4	8	7	0	64	68	4	1	-10	1	104	96	4	3	-5	1	614	624	3
5	-7	0	40	42	2	9	-11	0	31	33	3	1	-9	1	170	166	4	3	-4	1	122	130	4
5	-5	0	76	74	4	9	-6	0	106	109	4	1	-8	1	85	81	3	3	-3	1	214	219	3
5	-4	0	174	168	3	9	-5	0	38	36	3	1	-7	1	114	109	4	3	-2	1	54	54	2
5	-3	0	157	152	3	9	-2	0	35	32	5	1	-5	1	379	374	3	3	-1	1	433	440	3
5	-2	0	199	194	6	9	-1	0	205	207	5	1	-4	1	668	682	3	3	0	1	567	572	3

Appendix B

$2^2,6^5$-Diphenyl-p-septiphenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
3	4	1	283	274	4	6	-14	1	54	56	3	9	6	1	69	69	3	1	8	2	58	55	2
3	5	1	308	307	4	6	-13	1	103	106	4	10	-13	1	35	35	4	1	9	2	77	80	3
3	6	1	30	32	3	6	-11	1	61	60	3	10	-6	1	28	29	3	1	13	2	29	15	4
3	13	1	25	7	4	6	-9	1	143	152	5	10	-1	1	144	145	6	2	-9	2	131	126	4
4	-14	1	38	40	3	6	-8	1	143	140	5	10	0	1	52	51	2	2	-8	2	34	34	2
4	-13	1	118	125	5	6	-7	1	32	29	3	10	3	1	42	42	3	2	-7	2	37	40	2
4	-12	1	106	108	4	6	-6	1	101	95	3	10	5	1	76	78	3	2	-5	2	75	81	3
4	-10	1	47	45	2	6	-5	1	62	63	3	11	-12	1	31	19	4	2	-4	2	179	161	3
4	-9	1	61	55	3	6	-4	1	87	81	4	11	-8	1	37	41	4	2	-3	2	297	295	3
4	-8	1	274	272	4	6	-3	1	76	73	3	11	-6	1	24	20	4	2	-2	2	182	172	3
4	-7	1	107	110	4	6	-2	1	84	87	3	11	-4	1	55	55	3	2	-1	2	46	49	2
4	-6	1	214	209	4	6	-1	1	56	58	3	11	-3	1	79	86	5	2	0	2	84	83	3
4	-5	1	156	155	4	6	0	1	42	40	2	11	-2	1	29	26	4	2	1	2	31	26	2
4	-4	1	131	132	4	6	1	1	21	21	3	11	-1	1	56	54	2	2	2	2	43	46	2
4	-2	1	153	155	3	6	2	1	43	39	2	11	1	1	36	39	3	2	4	2	50	43	2
4	-1	1	156	152	3	6	3	1	27	23	3	12	-8	1	37	33	4	2	5	2	24	29	3
4	0	1	17	19	3	6	6	1	26	28	4	12	-2	1	38	40	3	2	6	2	187	186	4
4	1	1	84	74	4	6	7	1	80	77	3	13	-5	1	58	57	3	2	7	2	68	69	3
4	2	1	363	350	3	6	8	1	59	64	3	13	-4	1	117	111	4	2	8	2	82	82	4
4	3	1	115	111	4	6	9	1	28	31	4	0	0	2	101	99	3	2	9	2	82	79	3
4	4	1	95	92	3	7	-12	1	84	85	3	0	1	2	202	198	3	2	10	2	25	20	4
4	6	1	104	100	4	7	-10	1	36	35	3	0	2	2	60	54	2	2	11	2	29	31	4
4	7	1	80	82	3	7	-8	1	44	46	2	0	3	2	83	78	3	3	-12	2	83	81	4
4	8	1	98	101	4	7	-7	1	43	41	2	0	4	2	82	76	3	3	-11	2	77	83	3
4	9	1	84	83	3	7	-6	1	154	145	5	0	5	2	39	42	2	3	-10	2	123	125	5
4	10	1	42	42	3	7	-5	1	66	67	2	0	6	2	106	102	4	3	-9	2	88	92	5
4	11	1	88	86	2	7	-3	1	30	25	3	0	7	2	121	119	4	3	-8	2	53	53	2
4	12	1	65	68	3	7	-2	1	25	32	3	0	8	2	138	134	5	3	-7	2	416	420	4
5	-13	1	32	33	3	7	3	1	36	35	3	0	9	2	164	160	5	3	-6	2	214	209	4
5	-11	1	227	222	5	7	4	1	40	35	3	0	10	2	89	94	3	3	-5	2	68	66	2
5	-10	1	115	110	4	7	5	1	69	68	3	0	12	2	56	57	3	3	-4	2	43	43	2
5	-9	1	99	106	4	7	6	1	90	85	4	1	-11	2	21	21	5	3	-3	2	208	207	3
5	-8	1	42	42	2	7	7	1	91	96	5	1	-10	2	27	34	4	3	-2	2	364	381	3
5	-7	1	123	117	5	8	-14	1	31	33	4	1	-9	2	41	40	2	3	-1	2	262	273	3
5	-6	1	390	396	4	8	-12	1	57	58	2	1	-8	2	46	41	2	3	0	2	100	100	4
5	-5	1	143	148	4	8	-9	1	31	30	3	1	-7	2	76	70	3	3	1	2	73	76	3
5	-4	1	34	32	2	8	-7	1	48	44	2	1	-6	2	44	38	3	3	2	2	126	123	4
5	-2	1	44	46	2	8	-1	1	27	25	3	1	-5	2	40	35	2	3	3	2	19	16	4
5	-1	1	129	125	4	8	0	1	148	144	5	1	-4	2	42	44	2	3	4	2	112	110	4
5	0	1	118	126	4	8	5	1	108	109	5	1	-3	2	143	147	3	3	5	2	32	34	3
5	1	1	166	162	4	8	6	1	88	92	4	1	-2	2	347	349	3	3	6	2	63	66	2
5	2	1	106	97	4	8	7	1	36	30	3	1	-1	2	472	476	3	3	7	2	50	51	3
5	4	1	24	11	3	9	-6	1	28	20	4	1	0	2	291	281	3	3	8	2	95	96	4
5	5	1	55	52	3	9	-3	1	52	53	2	1	1	2	244	238	3	4	-15	2	30	33	4
5	6	1	66	64	3	9	-1	1	30	30	3	1	2	2	181	172	3	4	-10	2	150	155	5
5	7	1	56	57	2	9	0	1	53	55	3	1	3	2	212	212	4	4	-9	2	220	223	5
5	8	1	26	29	4	9	3	1	58	58	3	1	4	2	58	65	2	4	-8	2	68	67	3
5	9	1	131	133	5	9	5	1	83	84	4	1	6	2	35	34	2	4	-7	2	51	53	2

$2^2,6^5$-Diphenyl-p-septiphenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
4	-6	2	82	81	4	6	9	2	70	70	2	11	0	2	30	31	4	3	-11	3	73	75	2
4	-5	2	91	89	3	7	-14	2	82	83	2	12	-7	2	22	5	5	3	-10	3	83	78	3
4	-4	2	307	303	3	7	-13	2	206	213	6	0	0	3	340	327	3	3	-9	3	112	111	4
4	-3	2	51	53	2	7	-12	2	47	47	2	0	1	3	205	192	4	3	-8	3	96	97	3
4	-2	2	78	81	3	7	-11	2	68	69	2	0	2	3	93	92	3	3	-6	3	21	15	4
4	-1	2	28	32	3	7	-10	2	33	29	3	0	4	3	34	38	3	3	-5	3	57	53	2
4	0	2	401	403	3	7	-9	2	72	73	3	0	5	3	107	108	4	3	-4	3	194	190	4
4	2	2	35	34	2	7	-8	2	82	78	3	0	6	3	47	52	2	3	-3	3	384	372	4
4	4	2	57	61	5	7	-7	2	86	84	3	0	7	3	52	50	2	3	-1	3	101	103	4
4	5	2	93	91	4	7	-6	2	64	62	3	0	8	3	91	91	4	3	1	3	24	10	3
4	6	2	40	38	3	7	-5	2	28	22	3	0	9	3	168	162	5	3	2	3	97	99	4
4	7	2	60	62	2	7	-4	2	41	43	2	0	10	3	167	174	6	3	3	3	53	44	2
4	8	2	57	55	3	7	-3	2	133	127	5	0	11	3	42	47	3	3	6	3	70	77	2
4	9	2	34	30	3	7	4	2	27	25	4	1	-12	3	145	149	5	4	-13	3	56	52	3
5	-14	2	25	27	4	7	5	2	49	52	2	1	-11	3	106	114	4	4	-12	3	66	65	2
5	-12	2	44	40	3	7	6	2	23	31	4	1	-10	3	89	87	3	4	-11	3	62	66	4
5	-11	2	34	27	3	7	7	2	92	92	4	1	-9	3	68	70	3	4	-10	3	75	77	2
5	-10	2	100	100	3	7	9	2	25	17	5	1	-8	3	31	36	3	4	-9	3	28	30	4
5	-9	2	53	50	2	8	-13	2	85	84	3	1	-4	3	18	18	4	4	-7	3	42	38	2
5	-8	2	134	137	4	8	-12	2	62	55	2	1	-3	3	128	130	4	4	-6	3	49	49	3
5	-7	2	174	170	4	8	-11	2	78	80	3	1	-2	3	138	145	4	4	-5	3	71	66	2
5	-6	2	85	79	4	8	-9	2	25	19	4	1	-1	3	82	86	3	4	-4	3	111	109	4
5	-5	2	56	52	2	8	-7	2	46	41	3	1	1	3	22	15	3	4	-2	3	183	189	4
5	-4	2	30	32	3	8	-6	2	174	177	5	1	2	3	167	160	4	4	-1	3	169	170	4
5	-3	2	361	350	4	8	-4	2	48	48	3	1	3	3	24	31	3	4	3	3	127	125	5
5	-2	2	335	334	4	8	-2	2	25	21	4	1	6	3	70	71	3	4	4	3	191	206	5
5	-1	2	60	59	3	8	1	2	25	22	4	1	7	3	280	289	5	5	-12	3	29	32	4
5	0	2	38	33	2	8	3	2	50	49	3	1	8	3	178	184	6	5	-10	3	73	73	4
5	1	2	75	71	3	8	4	2	63	73	2	1	9	3	54	53	2	5	-9	3	135	129	5
5	2	2	103	105	4	9	-12	2	27	22	4	1	11	3	29	22	4	5	-6	3	77	70	3
5	3	2	115	110	4	9	-9	2	76	76	2	2	-15	3	48	51	3	5	-4	3	138	148	5
5	5	2	66	63	2	9	-8	2	64	65	3	2	-12	3	35	33	3	5	-3	3	106	99	5
5	6	2	70	70	2	9	-7	2	72	76	2	2	-6	3	44	44	2	5	-2	3	108	106	5
5	7	2	61	64	3	9	-4	2	22	26	4	2	-5	3	189	179	4	5	1	3	137	133	5
5	8	2	44	40	3	9	-1	2	29	28	3	2	-4	3	127	128	4	5	2	3	48	47	2
6	-15	2	30	30	4	9	0	2	67	65	2	2	-3	3	59	62	2	5	3	3	85	81	3
6	-13	2	58	60	2	9	1	2	56	61	3	2	-2	3	23	25	3	5	5	3	33	30	3
6	-12	2	101	99	3	9	5	2	64	65	3	2	-1	3	238	224	4	6	-13	3	48	49	3
6	-11	2	207	214	5	10	-3	2	26	24	4	2	0	3	125	142	4	6	-11	3	77	81	3
6	-10	2	189	190	5	10	-2	2	87	84	3	2	1	3	36	33	2	6	-10	3	50	49	3
6	-8	2	54	57	3	10	0	2	33	32	3	2	2	3	58	51	2	6	-7	3	25	28	4
6	-5	2	113	107	4	10	2	2	43	42	3	2	3	3	27	22	3	6	-4	3	39	41	3
6	-4	2	37	35	2	10	3	2	97	90	3	2	4	3	130	144	5	6	-3	3	142	138	5
6	-3	2	61	65	2	10	4	2	36	44	4	2	5	3	162	166	5	6	-2	3	144	149	5
6	-1	2	22	13	3	10	5	2	39	39	3	2	7	3	77	71	2	6	0	3	26	24	4
6	0	2	173	164	4	11	-4	2	25	29	4	2	8	3	75	74	2	6	2	3	30	34	4
6	1	2	54	55	2	11	-2	2	32	29	3	3	-13	3	31	22	3	6	3	3	49	54	2
6	5	2	26	20	4	11	-1	2	25	30	5	3	-12	3	46	52	3	7	-13	3	58	56	3

Values of 10*Fobs and 10*Fcalc

$2^2,6^5$-Diphenyl-p-septiphenyl

H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF	H K L	Fobs	Fcalc	SigF
7-11 3	42	40	3	2 -1 4	96	95	2	5 4 4	53	54	3	3 -7 5	23	23	5
7-10 3	32	31	3	2 0 4	76	76	3	6 -9 4	25	29	4	3 -6 5	24	15	4
7 -7 3	25	28	4	2 2 4	127	124	5	6 -8 4	38	39	3	3 -4 5	42	47	3
7 -5 3	128	132	5	2 3 4	176	170	5	6 -6 4	34	31	3	3 -3 5	68	73	3
7 -4 3	99	108	6	2 5 4	29	36	4	6 -5 4	44	46	3	3 -2 5	62	67	3
7 -3 3	76	74	2	2 7 4	118	124	5	6 -4 4	150	155	6	3 -1 5	58	65	3
7 -1 3	28	22	4	2 8 4	112	105	4	6 -3 4	200	206	5	3 0 5	25	24	5
7 4 3	26	20	4	3-15 4	66	69	4	6 -2 4	63	65	2	3 2 5	25	28	5
8-13 3	140	139	5	3 -9 4	23	20	5	6 -1 4	55	54	2	4-12 5	24	20	5
8-12 3	72	73	2	3 -5 4	129	121	4	6 1 4	122	115	5	4 -4 5	29	16	4
8 -9 3	31	29	3	3 -4 4	57	57	2	6 2 4	106	108	4	4 0 5	119	119	5
8 -8 3	34	34	3	3 -3 4	70	74	4	6 3 4	36	39	4	4 1 5	83	83	3
8 -4 3	28	29	4	3 -2 4	63	61	2	6 6 4	40	35	3	4 3 5	26	29	5
8 -3 3	23	19	4	3 0 4	150	157	6	7 -6 4	60	64	3	4 5 5	54	51	3
8 6 3	27	23	5	3 1 4	51	51	3	7 -4 4	121	120	4	5 -8 5	53	53	3
9-13 3	69	73	2	3 2 4	62	62	3	7 -3 4	51	57	3	5 -7 5	44	43	3
9 -6 3	80	82	3	3 3 4	27	24	4	7 -2 4	34	38	3	5 -4 5	28	34	4
9 3 3	27	35	4	3 4 4	68	64	3	7 -1 4	59	57	2	5 -2 5	107	110	4
10 -9 3	61	62	2	3 5 4	187	181	5	7 1 4	27	27	4	5 2 5	37	38	4
10 -8 3	92	95	4	3 6 4	37	30	3	7 3 4	69	70	2	6-11 5	39	35	3
10 -6 3	47	39	4	3 9 4	75	73	3	8-10 4	34	29	4	6-10 5	105	103	4
10 -5 3	29	28	4	4-11 4	23	25	4	8 -9 4	30	26	4	6 -4 5	47	49	3
10 -4 3	43	35	3	4 -8 4	154	159	6	8 -6 4	33	33	3	6 -2 5	24	28	5
10 -3 3	29	29	4	4 -7 4	75	71	3	8 -4 4	59	67	3	6 -1 5	46	54	3
10 1 3	50	50	3	4 -6 4	41	37	3	8 -3 4	43	45	3	6 0 5	63	62	3
10 2 3	29	25	4	4 -4 4	35	43	3	8 -2 4	33	30	4	7-10 5	41	45	3
11 -9 3	30	25	4	4 -3 4	137	136	5	9 1 4	29	17	4	7 -6 5	27	10	5
11 -2 3	66	67	5	4 -1 4	50	55	3	10 -6 4	43	34	3	7 -4 5	90	100	5
11 -1 3	49	54	4	4 0 4	25	15	4	10 -5 4	48	47	3	7 -3 5	158	163	6
0 0 4	57	59	2	4 1 4	32	35	4	0 0 5	68	72	3	7 -2 5	41	39	3
0 1 4	36	33	3	4 2 4	147	159	5	0 1 5	61	63	2	8 -6 5	132	128	4
0 3 4	50	56	3	4 3 4	49	41	2	1-11 5	60	61	2	8 -5 5	108	101	4
0 9 4	49	43	3	4 5 4	35	31	3	1-10 5	54	56	3	8 -4 5	81	87	3
1-11 4	54	52	2	4 6 4	59	57	2	1 -6 5	42	43	3	0 1 6	48	48	3
1 -9 4	71	71	2	4 7 4	70	62	3	1 -5 5	48	51	3	1-10 6	58	60	3
1 -7 4	33	38	3	5-11 4	54	57	2	1 -3 5	67	71	3	1 -7 6	61	62	4
1 -6 4	26	23	4	5-10 4	88	94	4	1 -2 5	73	73	3	1 -3 6	66	71	2
1 -4 4	30	26	3	5 -9 4	28	26	4	1 -1 5	37	39	3	1 -1 6	28	26	4
1 0 4	97	88	4	5 -8 4	38	39	3	1 0 5	37	36	3	2 -8 6	38	35	4
1 1 4	101	103	4	5 -6 4	97	99	5	1 4 5	25	26	5	2 -5 6	75	76	2
1 4 4	31	27	4	5 -5 4	71	74	3	2-13 5	54	51	3	2 -3 6	33	33	4
1 5 4	80	87	2	5 -4 4	54	49	4	2-10 5	32	30	4	3 -8 6	30	34	5
1 10 4	42	41	3	5 -3 4	132	131	4	2 -9 5	36	30	3	3 -4 6	31	29	4
2-15 4	30	24	4	5 -2 4	113	117	5	2 -8 5	39	37	3	3 1 6	41	42	4
2-12 4	110	107	4	5 -1 4	144	141	6	2 -1 5	44	39	3	3 2 6	35	35	5
2 -4 4	37	35	3	5 0 4	122	128	5	2 4 5	32	32	4	4 -9 6	27	11	5
2 -3 4	88	91	3	5 1 4	46	46	3	2 6 5	77	78	3	4 -1 6	37	36	4
2 -2 4	40	35	3	5 3 4	22	14	5	2 7 5	49	45	3	4 1 6	27	25	5

Appendix B

$2^2,6^5$-Diphenyl-p-septiphenyl

Values of 10*Fobs and 10*Fcalc

H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF	H	K	L	Fobs	Fcalc	SigF
1	-4	7	43	43	4																		

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